

APPENDIX C

COMBUSTION CATALYSTS FOR TURBINES

Introduction

I described possible alternative combustion catalyst configurations and detailed analysis of relevant performance factors, i.e., mass-transfer limited hydrocarbon conversions, pressure drop, catalyst temperatures, post combustion conversion of hydrocarbons and CO, etc. This report represents a comprehensive collection of my findings and comments. Attached are the final MathSoft Mathcad 6 analyses of the suggested alternative combustion catalyst configurations.

Alternative Combustion Catalyst Configurations

Two approaches are suggested for the catalytic combustion of gasoline vapors in air. These approaches represent more conventional and perhaps less expensive alternatives to the PCI Microlith™ technology. They are summarized as follows:

- **Monolith with bypass air** -- A standard 3.5", corrugated FeCrAl alloy, 600 cells/in² monolith should be able to reach $\approx 86\%$ (naphtha) to $>99.8\%$ (natural gas) fuel conversions. Using an air by-pass would allow longer residence time and higher adiabatic temperature rise (which is probably necessary for natural gas but may not be for diesel fuel or naphtha) within the combustor to ensure fast catalytic reaction rates. Higher temperatures within and at the exit of the catalyst monolith would also increase homogeneous combustion reactions, and help convert residual fuel vapors in the region immediately downstream of the catalyst but upstream of the turbine. A controller for bypass flow could help with turn-down, startup, and tuning steady-state conversions.
- **Radial flow catalyst bed** -- Provided that the flow rate can be reduced to < 3 m/s, a thin packed bed of catalyst beads or granules may also achieve conversions similar to those of the monolith and PCI Microlith™ catalyst screens at equivalent pressure drop. The bed might intrude upon your fuel injection and premixing zone, but this could actually benefit combustion (within limits, e.g., $\pm 30\%$ fuel/air ratio) by providing locally higher adiabatic temperatures. A packed bed has fairly good thermal conductivity and is virtually immune to thermal shock problems. A screened frame and possibly metal plates (or alternatively for robustness, silica-coated silicon carbide) could be located within the bed to guide the flow. Downstream hydrocarbon and CO conversion also would be necessary for low emissions as in the case of the monolith.

- **Exhaust converter** -- A 400 cells/in² post combustion monolith located just ahead of the regenerator exhaust stream inlet could provide a very significant reduction in hydrocarbon emissions regardless of the configuration and performance of the combustion catalyst. An emission control monolith should remove about 99% of the residual unburned fuel components and > 99.9% of the CO.

Analysis of Catalyst Performance

Mathsoft's Mathcad 6.0 Plus Professional program was used to perform detailed calculations of pressure drop and conversion of C₁, C₅, C₇, and C₉ hydrocarbons (methane, isopentane, cycloheptane and nonene) and CO. The analyses generally assume catalytic rates are fast under Capstone's specified combustion conditions. The analyses use various catalyst parameters such as particle/channel size and bed length for the two upstream (monolith and fixed bed) configurations. Only monoliths were considered for the downstream 1-atm conversion of residual CO and hydrocarbons.

Gas Properties

Initially the Mathcad document describes and defines various gas component and mixture properties and functions (pp. 1-13) that are used in the subsequent calculations. The gas and vapor components are identified with their physical parameters (p. 1) and the composition of combustion mixtures as a function of fuel conversion are defined (pp. 2-3). Mixture densities, diffusivities of individual fuel component in the mixtures, viscosity, and thermal conductivity are then defined and plotted as functions of composition and temperature (pp. 4-9). The composition of various fuel mixtures is shown to minimally effect mixture physical properties (< 0.5% under such lean conditions). These properties are then redefined as empirical functions of temperature for simplification of subsequent analysis (pp. 6-9). Heat capacities, heats of combustion and enthalpy functions of the mixtures are similarly defined (pp. 9-11), and the initial composition necessary for

an adiabatic temperature rise of 511°F are determined for each of the four fuel components (p. 11 and re-entered on p. 2). Finally, transport functions, e.g., Prandtl Number, Schmidt Number, thermal diffusivity, momentum diffusivity, etc., are defined (pp. 12-13) prior to definitions of the catalyst configurations, geometry, and flow conditions.

Catalyst Configurations

The physical parameters of several catalyst configurations (honeycomb monoliths and packed beds) and the appropriate flow conditions are described (p. 14) and used in the subsequent analyses.

Combustion Monolith Performance

The pressure drop values for (standard) 3.5 or 4.0 inch length 400 and 600 cells/in² monoliths are determined as functions of flow rate (pp. 15-16, and see figure on p. 16). Heat and mass Nusselt functions are defined and used to calculate single-pass fuel conversion vs. monolith depth (p. 17-19). It is possible to determine laminar flow hydrothermal Nusselt functions for square or sinusoidal channels (which may be more representative of actual monolith channel shapes), but this was not included in the current analysis. Accordingly the Nusselt functions cannot be considered more accurate than about $\pm 30\%$.

The results of the performance analysis for the monoliths are summarized in a table (p. 18) for the two cell densities, the two lengths, and 0, 20, and 40% by-pass air. The transport-limiting conversion of fuel components is plotted as a function of pressure drop for constant flow rate but extended monolith length (p. 19). High fuel conversions ($\approx 99.5\%$) are possible with the 600 cells/in² monolith at 1% pressure drop (but it requires 10 inches length).

Post Combustion Converter

Analysis of post-combustion downstream (1-atm vs. 3-atm upstream) conversion of CO and fuels and the pressure drop in 400 and 600 cpi monoliths shows excellent results for such a wide area monolith (pp. 20-25). After defining component diffusivity functions and describing monolith configuration (pp. 20-21), the pressure drop and conversions of CO and fuel vapors are calculated and plotted as functions of monolith depth (pp. 21-23). Finally, the results of an analysis of the overall conversions of individual hydrocarbons and CO including upstream combustor, homogeneous combustion, and the exhaust converter are tabulated (p. 23).

Differential (Local) Nusselt Analysis

A different analysis, where the local hydrothermal Nusselt functions are defined and integrated over the length of a monolith (pp. 24-25), are used to check the integral formulas.

These values (p. 25), which are derived from different sources (Kays and Crawford, "Convection Heat and Mass Transfer," 3rd, 1993, vs. Rosner, "Transport Processes in Chemically Reacting Systems", 1986) show higher conversions than the integrated values, e.g., 94% conversion for C_7H_{14} vs. 86% with the integral expression. This difference appears to be caused by the greater effect of hydrothermal entrance (as opposed to hydrodynamically developed flow with thermal entrance) and shows the integral formulas to be conservative by a factor of about two.

Combustion with Packed Beds

Pressure drop and fuel conversion functions are defined and used to analyze the performance of packed beds (pp. 26-31). Pressure drop is a strong function of the superficial flow rate, nearly second order (pressure drops are calculated and plotted against superficial linear flow velocity for various sizes of catalyst particles on p. 27). Gas to particle Nusselt numbers for packed beds are developed plotted for methane, isopentane, cycloheptane and nonene for three sizes of catalyst granules (pp. 27-28). Shape factors are not included in this analysis, so the results represent values for packed spheres with equivalent effect on ΔP , not with equivalent diameter. The conversion of fuel components (again assuming very fast catalytic rates) is determined (pp. 28-29) for the oblique flow geometry (which is defined on p. 16).

For full perpendicular flow such as with an annular cylindrical packed bed rather than the conical bed, the pressure drop function is much greater for equivalent conversion of fuel components. This is caused by the higher power dependence of ΔP on flow velocities (form drag), while the conversion per unit depth of bed increases almost linearly with increasing flow rate. At flows higher than about 2 m/s the catalyst granules begin to act as bluff bodies which cause the flow to accelerate around them. While this increases backmixing which helps convection, it causes a greater effect on the pressure drop. Conversions for methane and cycloheptane are plotted as a function of pressure drop for beds of 1-mm and 1/8-in. granules (pp. 29-31). For oblique flow (2.5 m/s superficial velocity through the conical bed) with the small granules, C_7H_{14} conversions are calculated to be very high ($> 99.99\%$) at 1% pressure drop, while for perpendicular flow (8.2 m/s) with the 1/8-in. pellets, C_7H_{14} conversions are calculated to be very low ($\approx 62\%$) at 2% pressure drop. Clearly some radial configuration must be used to achieve high conversions with the packed beds without a pressure drop penalty.

Required Catalytic Rates

Finally, the specific catalytic rate constants required for conversions of methane and cycloheptane in a 600 cells/in² monolith are determined (pp. 32-35) for Capstone's conditions.

The effect of gas diffusional restrictions within the macroporous (pores between agglomerated washcoat particles within a catalyst layer) and microporous (within the porous particles) is defined for CH_4 and C_7H_{14} (pp. 32-33). The effect of rate constant on surface temperature (for a point at the entry to the channel) is determined (p. 34) and shows the rates necessary to move fully into the transport limited regime, i.e., when the concentration of fuel near the surface approaches zero and temperature approaches a limit. This analysis could be turned around by calculating the conversion for a given catalytic rate constant.

But, further analysis of the expected conversions requires measurements of the actual rate of the washcoated catalysts and catalyst beds. The analysis concludes with a complex rate expression for methane combustion by supported PdO that was based on measured rates (in the absence of transport limitations). This rate was based on PdO , an hexa-aluminate support ($\text{LaAl}_{11}\text{O}_{18}$) with a much lower surface area than the La-stabilized supported used in the Capstone monoliths and pellets. The interception of the curve showing the surface temperature as a function of catalytic rate constant (as on p. 35) and the curve showing the actual rate constant of the catalyst as a function of catalyst temperature (plotted on p. 37) given the actual performance of the catalyst.

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More detailed calculations would integrate the conversion through the monolith or packed bed and it would include the thermal conduction along the monolith channel or within the bed. This would represent a one-dimensional calculation (axial surface and gas phase temperatures) which is only an approximation to the actual two- or three-dimensional convective transport and reaction problem. Such calculations could provide estimates of extinction conditions for specific catalysts. Such calculations and further analyses are beyond the scope of the current comments, but could be performed by extending the current Mathcad 6 program.

Conclusions

Catalyst Performance

Several conclusions can be drawn about the transport limiting performance of a catalysts used to combustion gasoline and methane fuels for Capstone's 24 kW microturbine:

- 1) Commercially available small cell (600 cells/in²) honeycomb monoliths should be seriously considered as an alternative to the PCI Microlith technology. A catalytic monolith configured as annular flow 600 cells/in² honeycomb can achieve very high conversion of methane (99.99%) and
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modest conversion for gasoline (94% for cycloheptane) etc. with low pressure drop.

- 2) If the fuel air mixing can be moved upstream sufficiently to allow use of a longer catalyst monoliths, significantly lower emission could result without unacceptable ($> 1\%$) pressure drop ratio. For $1\% \Delta P/P$ drop (with greater monolith length), transport limited conversion of C_7H_{14} should reach 99.5% in an active 600 cells/in² honeycomb monolith.
- 3) Post combustion monolith catalysts should be considered for use in EZEVE turbines, regardless of the method of fuel conversion during combustion. A short 400 cells/in² Alpha-IV metal monolith coated with a layer of supported Pt located at the inlet to the recuperator can give very significant emission reductions for CO and all hydrocarbons because of the lower linear velocities, high exhaust temperature, greater diffusivities at 1-atm. Conversions of CO and CH_4 can be very high, while conversions with C_7H_{14} and other gasoline fuels is less, it still can bring the gasoline range fuel components in the exhaust to a few ppm with the assumption that only a modest degree of homogeneous combustion occurs upstream of the turbine.
- 4) Provided that significant homogeneous combustion occurs within the channels and downstream of the monolith ($\approx 80\%$ conversion giving 60 ppm C_7H_{14} and 840 ppm CO leaving the turbine) and that a 400 cells/in² post combustion hydrocarbon oxidation catalyst was used downstream, gasoline emissions should fall below 0.5 ppm.
- 5) The oblique flow/conical catalyst packed bed could also be considered as an option to the MicrolithTM and honeycomb monolith catalysts. The performance of the packed beds can be very good in terms of fuel conversion with the smaller catalyst granules. Yet, these beds must have some element of radial flow as the pressure drop for a flow linear flow rate will cause excessive pressure drop. A word of caution here, packed beds are more susceptible to flash back caused by the higher degree of backmixing and regions where local residence times can be quite long relative to the screens and monoliths.

Catalyst Durability, Robustness, and Costs

- 1) [REDACTED] concerns were expressed about the tolerance of combustion catalysts to momentarily high fuel/air ratios and local unmixedness. While clearly high degrees of F/A control and uniformly premixed combustion gases are desired, the combustion catalysts should show robustness sufficient to survive short excursions of off-specification F/A ratio conditions as well as showing the durability necessary for long active life under normal operation at high temperatures.
- 2) The greater the thermal mass of the catalyst, the greater its robustness in the face of locally or globally high F/A. In this regard the packed beds would be

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superior to the fine screens of the Microlith™ and the thin walled metal monoliths.

- 3) A packed bed also has greater ability to disperse locally high F/A mixtures to a greater extent than the Microlith™ and to a much greater than the honeycomb channels. High thermal conductivity also improves robustness in locally high F/A (hot spot) conditions. Here the packed bed is perhaps superior to the metal monolith because of its greater radial conductivity, while the screens have very little ability (radiation) to disperse heat from locally hot zones.
- 4) The Alpha-IV alloy honeycomb should be much more resistant to fast overheating to high temperatures than the PCI-microlith. The Alzeta/Grace electrically heated monolith previously examined by Capstone (Nomac) had entrance channels too large to give high conversion except with long length and smaller channels downstream, hence the large volume and weight.
- 5) Packed beds represent the least cost catalyst for combustion because they use configurations and materials common with commercial VOC incineration catalysts. The metal monoliths have low costs because of their widespread acceptance and increasing use in automobile catalytic converters and as VOC catalysts. The premixed, gasoline-fueled, and recuperated nature of the combustion process for Capstone's microturbines is a good fit (with a slight push to higher pressure, higher throughput, low pressure drop, and greater robustness) with the commercial VOC catalysts available from several sources, including Prototech/United Catalysts. It would not appear necessary to develop new catalyst and catalytic engineered combustors for Capstone' microturbine combustion applications.

The following table summarizes the findings of this analysis:

Property	Ranking		
Fuel Conversion	Packed Beds >	Screens >	Monoliths
Pressure Drop	Monoliths >	Screens >	Packed Beds
Durability	Packed Beds ≈	Monoliths ≈	Screens
Robustness	Packed Beds >	Monoliths >	Screens
Cost & Availability	Packed Beds >	Monoliths >	Screens

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Final Recommendations

Use of Catalysts in Existing Engines

The following recommendations are made on the basis of improving the *existing* microturbine catalytic combustion performance:

- 1) Install 400 cells/in² 1-atm monolith with a Pt-based catalyst for post combustion CO and hydrocarbon removal. This unit should provide the greatest improvement in emissions with little effect on pressure drop at modest cost (\approx \$200/unit installed). It could be used with all catalytic and even with non-catalytic burners to reduce CO and hydrocarbon emissions. However, it cannot be effective in reducing NOx emissions from non-catalytic burners.
- 2) Use a 600 cells/in² Alpha-IV alloy metal monolith of 4-in. length with premixed fuel and air as a lower pressure drop alternative to the PCI Microlith™ system. Fuel conversion may be lower than the PCI unit, but with lower pressure drop; at equivalent $\Delta P/P$, the monolith should show superior fuel conversion. A small amount of by-pass air could help with turn-down and could be used to improve emissions during normal operation by increasing residence time and allowing higher temperatures in the homogeneous zones within the channels and immediately downstream of the combustor.

Use of Catalysts in Advanced Engines

For *advanced* combustion systems, the fuel air mixing could be moved upstream of its current position to allow great premixing and to give greater volume for the catalyst.

- 1) Nominally 1-mm to 1/16-in. packed beds in a conical configuration with about 2-3 m/s linear superficial bed velocity could give good performance, especially with a small bypass air stream for post catalyst hydrocarbon reduction. An inconel screen could be located upstream to suppress flashback and ceramic foams or honeycomb monoliths could be used as mechanical supports to increase robustness.
- 2) A longer 600 cells/in² Alpha-IV alloy metal monolith (from 3.5- to 8- or 10-in.) could also decrease hydrocarbon and CO emissions with acceptable $\Delta P/P$ by relocating the F/A mixing zone upstream.

Additional Catalytic R&D Activities

Additional Analysis -- Fuel combustion rates can be measured for specific catalysts under Capstone's combustion conditions. The rates can be incorporated in an extended analysis of

combustor performance for use in predicting fuel conversion, specifying required catalyst activity maintenance (e.g., Is it close to extinction at 1000°F inlet temperature?), and assisting in the design of current and next generation combustors (e.g., How much by-pass air is necessary? What are the limited on F/A ratios?, etc.).

Advanced Materials

more robust units could be developed with ceramic structural components and state-of-the-art catalysts capable of resisting short (a few seconds) temperature excursions to 3000°F (1650°C).

The attrition resistance and crush strength of the Norton SA 6576 catalyst pellets supplied to Capstone by SRI International also need improvement (their very large specific volume of macropores, while desirable, leads to poor mechanical strength), and other catalysts (e.g., 1.5-mm extruded, Pt-promoted, Mn-substituted hexa-aluminates) could be examined for activity and attrition resistance.

In the longer-term,

SRI could coat steels with chromium and aluminum (*in situ* preparation of FeCrAl alloy films) to prepare inexpensive, high-performance recuperators and monoliths for use in advanced higher temperature engines.

Systems -- Additional engineering analysis and catalyst preparation and testing could provide Capstone with cost effective assistance in the design of EZEV turbogenerators with alternative fuels such as LPG, CNG, and diesel for hybrid vehicles. LPG could be used in the current designs with combustion and exhaust converter monoliths; CNG could be used with combustion and exhaust converter monoliths, but with by-pass air to increase F/A ratios and catalyst temperatures; and diesel fuel could require upstream mixing with long combustion monoliths or conical beds and longer exhaust converter monoliths.

Appendix C

GAS-ONE.MCD

Gas Properties and Constants

$\text{cm} = 0.01 \cdot \text{m}$ $J = \text{kg} \cdot \text{m}^2 \cdot \text{sec}^{-2}$ $W = J \cdot \text{sec}^{-1}$ $\text{Pref} = 1 \cdot \text{atm}$
 $N = \text{kg} \cdot \text{m} \cdot \text{sec}^{-2}$ $\text{Pa} = N \cdot \text{m}^{-2}$ $\text{atm} = 101300 \cdot \text{Pa}$ $\mu\text{m} = 0.000001 \cdot \text{m}$
 $R = 8.3143 \cdot \frac{J}{K}$ $R_c = 8.3143 \cdot J \cdot \text{mole}^{-1} \cdot K^{-1}$

n	Gas	MolWt	$\sigma(\text{LJ})$	$\epsilon(\text{LJ})$
1	CH4	$MW_0 = 16.044 \cdot \text{gm}$	$\sigma_0 = 3.785 \cdot 10^{-10} \cdot \text{m}$	$\epsilon_0 = 148.6 \cdot K$
2	O2	$MW_1 = 31.999 \cdot \text{gm}$	$\sigma_1 = 3.464 \cdot 10^{-10} \cdot \text{m}$	$\epsilon_1 = 106.7 \cdot K$
3	N2	$MW_2 = 28.018 \cdot \text{gm}$	$\sigma_2 = 3.798 \cdot 10^{-10} \cdot \text{m}$	$\epsilon_2 = 71.4 \cdot K$
4	CO2	$MW_3 = 44.010 \cdot \text{gm}$	$\sigma_3 = 3.941 \cdot 10^{-10} \cdot \text{m}$	$\epsilon_3 = 195.2 \cdot K$
5	H2O	$MW_4 = 18.015 \cdot \text{gm}$	$\sigma_4 = 2.641 \cdot 10^{-10} \cdot \text{m}$	$\epsilon_4 = 809.1 \cdot K$

$Tb5 = 301 \cdot K$ $Tc5 = 460.4 \cdot K$ $Pc5 = 3.39 \cdot 10^6 \cdot \text{Pa}$ $Vc5 = 306$

6 C5H12
2-methyl-butane

$$\epsilon_5 = \frac{Tc5}{1.2593} \quad \sigma_5 = Vc5^{\frac{1}{3}} \cdot 10^{-10} \cdot \text{m}$$

$$MW_5 = 72.151 \cdot \text{gm} \quad \epsilon_5 = 365.59994 \cdot K \quad \sigma_5 = 6.73866 \cdot 10^{-10} \cdot \text{m}$$

$Tc7 = 572.2 \cdot K$ $Tb7 = 374.1 \cdot K$ $Pc7 = 3.47 \cdot 10^6 \cdot \text{Pa}$ $Vc7 = 368$

7 C7H14
methyl-cyclohexane

$$\epsilon_6 = \frac{Tc7}{1.2593} \quad \sigma_6 = Vc7^{\frac{1}{3}} \cdot 10^{-10} \cdot \text{m}$$

$$MW_6 = 98.189 \cdot \text{gm} \quad \sigma_6 = 7.1661 \cdot 10^{-10} \cdot \text{m} \quad \epsilon_6 = 454.37942 \cdot K$$

$Tc9 = 592 \cdot K$ $Tb9 = 420 \cdot K$ $Vc9 = 580$ $Pc9 = 2.34 \cdot 10^6 \cdot \text{Pa}$

8 C9H18
1-nonene

$$\epsilon_7 = \frac{Tc9}{1.2593} \quad \sigma_7 = Vc9^{\frac{1}{3}} \cdot 10^{-10} \cdot \text{m}$$

$$MW_7 = 126.243 \cdot \text{gm} \quad \sigma_7 = 8.33955 \cdot 10^{-10} \cdot \text{m} \quad \epsilon_7 = 470.10244 \cdot K$$

9 CO

$$\epsilon_8 = 91.7 \cdot K \quad \sigma_8 = 3.69 \cdot 10^{-10} \cdot \text{m}$$

$$MW_8 = 28.01 \cdot \text{gm}$$

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Define constants for transport integrals:

$$\sigma\mu_{a_0} := 1.16145$$

$$\sigma\mu_{b_0} := 0.14874$$

$$\sigma Da_0 := 1.06036$$

$$\sigma Db_0 := 0.1561$$

$$\sigma\mu_{a_1} := 0.52487$$

$$\sigma\mu_{b_1} := 0.7732$$

$$\sigma Da_1 := 0.193$$

$$\sigma Db_1 := 0.47635$$

$$\sigma\mu_{a_2} := 2.16178$$

$$\sigma\mu_{b_2} := 2.43787$$

$$\sigma Da_2 := 1.03587$$

$$\sigma Db_2 := 1.52996$$

$$\sigma Da_3 := 1.76474$$

$$\sigma Db_3 := 3.89411$$

Define transport integrals:

$$\Omega\mu(T) := \sigma\mu_{a_0} \cdot \exp\left[-\left(\sigma\mu_{b_0} \cdot \ln(T)\right)\right] + \sum_{i\mu=1}^2 \sigma\mu_{a_{i\mu}} \cdot \exp\left(-\sigma\mu_{b_{i\mu}} \cdot T\right) \quad \Omega\mu(3) = 1.0394$$

$$\Omega D(T) := \sigma Da_0 \cdot \exp\left[-\left(\sigma Db_0 \cdot \ln(T)\right)\right] + \sum_{i\mu=1}^3 \sigma Da_{i\mu} \cdot \exp\left(-\sigma Db_{i\mu} \cdot T\right) \quad \Omega D(3) = 0.95002$$

Set Inlet Conditions:

$$P := 3 \cdot \text{atm}$$

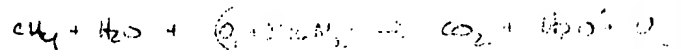
$$ych40 := 0.01183$$

$$y0c5h12 := 0.0028968$$

$$y0c7h14 := 0.0021859$$

$$y0c9h18 := 0.0016878$$

These values for y_{0i} have been determined via enthalpy functions on p. 11 for temperature rise from 1000F to 1511F.



Define gas composition w/r methane using moist (2%) air:

$$y(y0, x) := \begin{bmatrix} y0 \cdot (1 - x) \\ (1 - y0) \cdot 0.205 - 2 \cdot ych40 \cdot x \\ (1 - y0) \cdot 0.775 \\ y0 \cdot x \\ (1 - y0) \cdot 0.02 + 2 \cdot y0 \cdot x \\ 0 \\ 0 \\ 0 \end{bmatrix} \begin{matrix} \text{fuel} \\ O_2 \\ N_2 \\ CO_2 \\ H_2O \\ \\ \\ \end{matrix}$$

$$y(ych40, 0.1) = \begin{bmatrix} 0.0106 \\ 0.2002 \\ 0.7658 \\ 0.0012 \\ 0.0221 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$$\sum y(ych40, 0.5) = 1$$

$$(y_{fuel}, x)$$

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Define function for calculating stoichiometric gas composition for combustion of 2-methyl-butane using moist (2%) air:

$$C_5H_{12} \quad y_5(y_0, x) := \frac{\begin{bmatrix} 0 \\ (1-y_0) \cdot 0.205 - 8 \cdot y_0 \cdot x \\ (1-y_0) \cdot 0.775 \\ 5 \cdot (y_0 \cdot x) \\ (1-y_0) \cdot 0.02 + 6 \cdot y_0 \cdot x \\ y_0 \cdot (1-x) \\ 0 \\ 0 \end{bmatrix}}{1 + 2 \cdot y_0 \cdot x}$$

$\begin{matrix} C_5H_{12} \\ O_2 \\ N_2 \\ CO_2 \\ H_2O \\ C_5H_{12} \end{matrix}$

$$\sum y_5(y_0, x) = 1$$

$$y_5(y_0, x) = \begin{bmatrix} 0 \\ 0.192262 \\ 0.770523 \\ 0.007221 \\ 0.02855 \\ 0.001444 \\ 0 \\ 0 \end{bmatrix}$$

Define function for calculating stoichiometric gas composition for combustion of methyl-cyclohexane using moist (2%) air:

$$C_7H_{14} \quad y_7(y_0, x) := \frac{\begin{bmatrix} 0 \\ (1-y_0) \cdot 0.205 - 10.5 \cdot y_0 \cdot x \\ (1-y_0) \cdot 0.775 \\ 7 \cdot (y_0 \cdot x) \\ (1-y_0) \cdot 0.02 + 7 \cdot y_0 \cdot x \\ 0 \\ y_0 \cdot (1-x) \\ 0 \end{bmatrix}}{1 + 2.5 \cdot y_0 \cdot x}$$

$\begin{matrix} C_7H_{14} \\ C_5H_{12} \\ C_7H_{14} \end{matrix}$

$$\sum y_7(y_0, x) = 1$$

$$y_7(y_0, x) = \begin{bmatrix} 0 \\ 0.19255 \\ 0.771199 \\ 0.00763 \\ 0.027532 \\ 0 \\ 0.00109 \\ 0 \end{bmatrix}$$

Define function for calculating stoichiometric gas composition for combustion of 1-nonene using moist (2%) air:

$$C_9H_{18} \quad y_9(y_0, x) := \frac{\begin{bmatrix} 0 \\ (1-y_0) \cdot 0.205 - 13.5 \cdot y_0 \cdot x \\ (1-y_0) \cdot 0.775 \\ 9 \cdot (y_0 \cdot x) \\ (1-y_0) \cdot 0.02 + 9 \cdot y_0 \cdot x \\ 0 \\ 0 \\ y_0 \cdot (1-x) \end{bmatrix}}{1 + 3.5 \cdot y_0 \cdot x}$$

C_9H_{18}

$$\sum y_9(y_0, x) = 1$$

$$y_9(y_0, x) = \begin{bmatrix} 0 \\ 0.192692 \\ 0.771413 \\ 0.007573 \\ 0.02748 \\ 0 \\ 0 \\ 8.414148 \cdot 10^{-4} \end{bmatrix}$$

Define functions for evaluation of mixture properties (ideal gas) given fractional fuel conversion and temperature.

Density and average molecular weight:

$$\rho_{\text{mix}}(x, T) := \left(\sum_{kk=0}^7 y(\text{ych40}, x)_{kk} \cdot \text{MW}_{kk} \right) \cdot \frac{P}{R \cdot T} \quad \text{MW}_{\text{mix}}(x) := \left(\sum_{kk=0}^7 y(\text{ych40}, x)_{kk} \cdot \text{MW}_{kk} \right)$$

$$\rho_{\text{mix}}(1, 300\text{-K}) = 3.470573 \cdot \text{kg} \cdot \text{m}^{-3}$$

$$\text{MW}_{\text{mix}}(1) = 28.485 \cdot \text{gm}$$

Define diffusion coefficients for specific binary diffusion pairs:

$$\text{Diff}(n, m, T) := 1.8829 \cdot 10^{-27} \cdot \frac{\left[\left(\frac{1}{\text{MW}_n} + \frac{1}{\text{MW}_m} \right) \cdot T^3 \right]^{0.5}}{\left(\frac{\sigma_n + \sigma_m}{2} \right)^2 \cdot \Omega_D \left[\frac{T}{(\epsilon_n \cdot \epsilon_m)^{0.5}} \right] \cdot \frac{P}{P_{\text{ref}}}} \cdot 10^8 \cdot \text{gm}^{0.5} \cdot \text{cm}^4 \cdot \text{sec}^{-1} \cdot \text{K}^{-1.5}$$

$$\text{Diff}(0, 2, 300\text{-K}) = 0.07417 \cdot \text{sec}^{-1} \cdot \text{cm}^2$$

$$\text{Diff}(2, 7, 300\text{-K}) = 0.01597 \cdot \text{sec}^{-1} \cdot \text{cm}^2$$

Define functions for use with various fuel air mixtures:

$$\text{Dch4}(x, T) := \frac{1 - y(\text{ych40}, x)_0}{\sum_{j_{\text{gas}}=1}^7 \frac{y(\text{ych40}, x)_{j_{\text{gas}}}}{\text{Diff}(0, j_{\text{gas}}, T)}}$$

$$\text{Dch4}(0.5, 298\text{-K}) = 7.31327 \cdot 10^{-6} \cdot \text{m}^2 \cdot \text{sec}^{-1}$$

$$\text{Dc5h12}(x, T) := \frac{1 - y5(\text{y0c5h12}, x)_0}{\sum_{j_{\text{gas}}=1}^7 \frac{y5(\text{y0c5h12}, x)_{j_{\text{gas}}}}{\text{Diff}(5, j_{\text{gas}}, T)}}$$

$$\text{Dc5h12}(0.5, 298\text{-K}) = 2.28466 \cdot 10^{-6} \cdot \text{m}^2 \cdot \text{sec}^{-1}$$

$$\text{Dc7h14}(x, T) := \frac{1 - y7(\text{y0c7h14}, x)_0}{\sum_{j_{\text{gas}}=1}^7 \frac{y7(\text{y0c7h14}, x)_{j_{\text{gas}}}}{\text{Diff}(6, j_{\text{gas}}, T)}}$$

$$\text{Dc7h14}(0.5, 298\text{-K}) = 1.94254 \cdot 10^{-6} \cdot \text{m}^2 \cdot \text{sec}^{-1}$$

$$\text{Dc9h18}(x, T) := \frac{1 - y9(\text{y0c9h18}, x)_0}{\sum_{j_{\text{gas}}=1}^7 \frac{y9(\text{y0c9h18}, x)_{j_{\text{gas}}}}{\text{Diff}(7, j_{\text{gas}}, T)}}$$

$$\text{Dc9h18}(0.5, 298\text{-K}) = 1.53123 \cdot 10^{-6} \cdot \text{m}^2 \cdot \text{sec}^{-1}$$

Display gas mixture properties

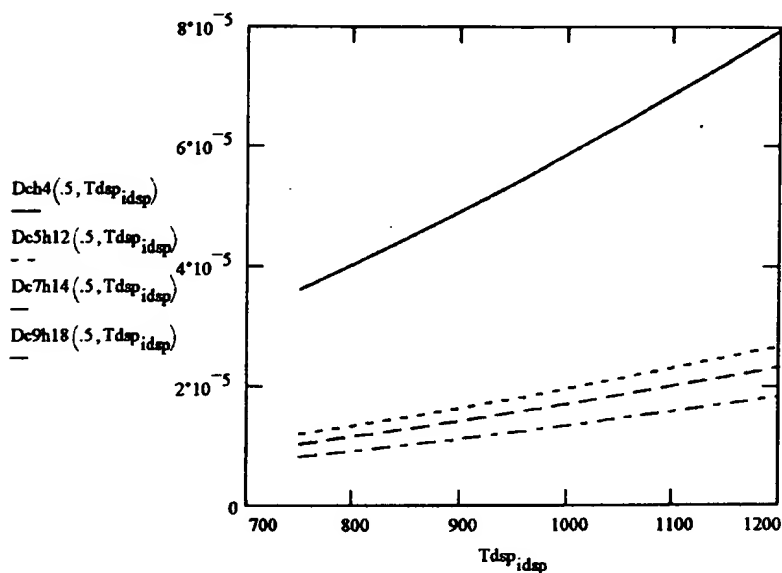
$$\text{idsp} := 0..9$$

$$T_{\text{dsp_idsp}} := (750 + 50 \cdot \text{idsp}) \cdot \text{K}$$

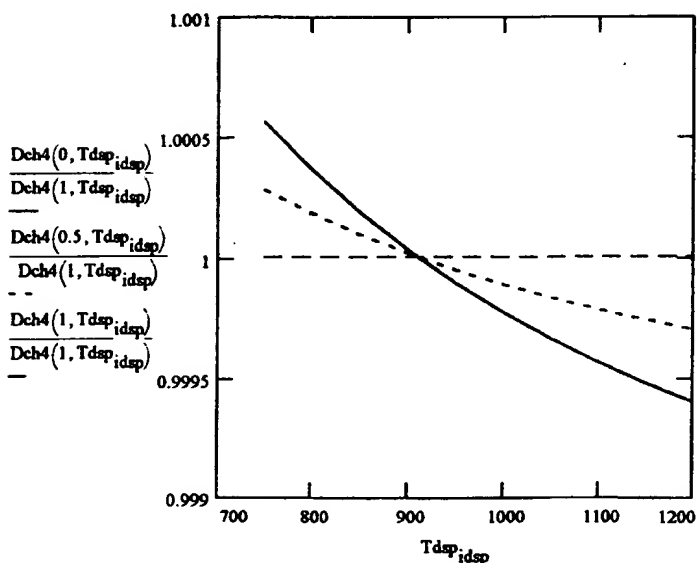
$$T_{\text{in}} := \left[(1000 - 32) \cdot \frac{5}{9} + 273.15 \right] \cdot \text{K} \quad T_{\text{in}} = 810.92778 \cdot \text{K} \quad T_{\text{out}} := \left[(1511 - 32) \cdot \frac{5}{9} + 273.15 \right] \cdot \text{K} \quad T_{\text{out}} = 1094.81667 \cdot \text{K}$$

Plots (below) of D_i for CH_4 , C_5H_{12} , etc. show large gap between CH_4 and the other hydrocarbons and show very little effect of fuel conversion (even for methane) on D_i because the fuels are so dilute.

Therefore we can choose methyl cyclohexane as the molecule representative of naphtha and ignore the effect of conversion on gas properties



$T_{\text{dsp_idsp}}$	$D_{\text{ch4}}(.5, T_{\text{dsp_idsp}})$
$7.5 \cdot 10^2 \cdot \text{K}$	$3.61119 \cdot 10^{-5} \cdot \text{m}^2 \cdot \text{sec}^{-1}$
$8 \cdot 10^2 \cdot \text{K}$	$4.02644 \cdot 10^{-5} \cdot \text{m}^2 \cdot \text{sec}^{-1}$
$8.5 \cdot 10^2 \cdot \text{K}$	$4.45884 \cdot 10^{-5} \cdot \text{m}^2 \cdot \text{sec}^{-1}$
$9 \cdot 10^2 \cdot \text{K}$	$4.90801 \cdot 10^{-5} \cdot \text{m}^2 \cdot \text{sec}^{-1}$
$9.5 \cdot 10^2 \cdot \text{K}$	$5.37357 \cdot 10^{-5} \cdot \text{m}^2 \cdot \text{sec}^{-1}$
$1 \cdot 10^3 \cdot \text{K}$	$5.85522 \cdot 10^{-5} \cdot \text{m}^2 \cdot \text{sec}^{-1}$
$1.05 \cdot 10^3 \cdot \text{K}$	$6.35265 \cdot 10^{-5} \cdot \text{m}^2 \cdot \text{sec}^{-1}$
$1.1 \cdot 10^3 \cdot \text{K}$	$6.8656 \cdot 10^{-5} \cdot \text{m}^2 \cdot \text{sec}^{-1}$
$1.15 \cdot 10^3 \cdot \text{K}$	$7.39384 \cdot 10^{-5} \cdot \text{m}^2 \cdot \text{sec}^{-1}$
$1.2 \cdot 10^3 \cdot \text{K}$	$7.93712 \cdot 10^{-5} \cdot \text{m}^2 \cdot \text{sec}^{-1}$



$T_{\text{dsp_idsp}}$	$D_{\text{c7h14}}(.5, T_{\text{dsp_idsp}})$
$7.5 \cdot 10^2 \cdot \text{K}$	$1.03475 \cdot 10^{-5} \cdot \text{m}^2 \cdot \text{sec}^{-1}$
$8 \cdot 10^2 \cdot \text{K}$	$1.15717 \cdot 10^{-5} \cdot \text{m}^2 \cdot \text{sec}^{-1}$
$8.5 \cdot 10^2 \cdot \text{K}$	$1.28482 \cdot 10^{-5} \cdot \text{m}^2 \cdot \text{sec}^{-1}$
$9 \cdot 10^2 \cdot \text{K}$	$1.41758 \cdot 10^{-5} \cdot \text{m}^2 \cdot \text{sec}^{-1}$
$9.5 \cdot 10^2 \cdot \text{K}$	$1.55533 \cdot 10^{-5} \cdot \text{m}^2 \cdot \text{sec}^{-1}$
$1 \cdot 10^3 \cdot \text{K}$	$1.69798 \cdot 10^{-5} \cdot \text{m}^2 \cdot \text{sec}^{-1}$
$1.05 \cdot 10^3 \cdot \text{K}$	$1.84541 \cdot 10^{-5} \cdot \text{m}^2 \cdot \text{sec}^{-1}$
$1.1 \cdot 10^3 \cdot \text{K}$	$1.99755 \cdot 10^{-5} \cdot \text{m}^2 \cdot \text{sec}^{-1}$
$1.15 \cdot 10^3 \cdot \text{K}$	$2.15429 \cdot 10^{-5} \cdot \text{m}^2 \cdot \text{sec}^{-1}$
$1.2 \cdot 10^3 \cdot \text{K}$	$2.31555 \cdot 10^{-5} \cdot \text{m}^2 \cdot \text{sec}^{-1}$

Define interpolation formulas for Dch4 and Dc7h14 vs. T(K) at x=0.5 via Jandel Scientific's Tablecurve program

$$Dch4T(T) := \exp\left(-11.718527 + 1.6257167 \cdot \ln\left(\frac{T}{K}\right) - \frac{46.77509 \cdot K}{T}\right) \cdot \frac{\text{cm}^2}{\text{sec}}$$

$$Dch4(.5, 1000 \cdot K) = 0.585522 \cdot \text{sec}^{-1} \cdot \text{cm}^2$$

$$Dch4T(1000 \cdot K) = 0.585523 \cdot \text{sec}^{-1} \cdot \text{cm}^2$$

$$Dc7h14T(T) := \exp\left(-12.923061 + 1.6260558 \cdot \ln\left(\frac{T}{K}\right) - \frac{82.480098 \cdot K}{T}\right) \cdot \frac{\text{cm}^2}{\text{sec}}$$

$$Dc7h14(.5, 1000 \cdot K) = 0.169798 \cdot \text{sec}^{-1} \cdot \text{cm}^2$$

$$Dc7h14T(1000 \cdot K) = 0.169798 \cdot \text{sec}^{-1} \cdot \text{cm}^2$$

Define viscosity functions for major constituents:

$$\mu(T) := \left[\frac{2.6693 \cdot 10^{-26} \cdot \left(\frac{MW_0 \cdot T}{\sigma_0^2 \cdot \Omega \mu \left(\frac{T}{\epsilon_0}\right)}\right)^{0.5} \cdot \frac{10^5 \cdot \text{cm}}{\text{sec}} \cdot \left(\frac{\text{gm}}{K}\right)^{0.5}}{\frac{(MW_1 \cdot T)^{0.5}}{(\sigma_1)^2 \cdot \Omega \mu \left(\frac{T}{\epsilon_1}\right)} \left[2.6693 \cdot 10^{-26} \cdot \left(\frac{10^5 \cdot \text{cm}}{\text{sec}}\right) \cdot \left(\frac{\text{gm}}{K}\right)^{0.5} \right]} \right. \\ \left. \frac{(MW_2 \cdot T)^{0.5}}{(\sigma_2)^2 \cdot \Omega \mu \left(\frac{T}{\epsilon_2}\right)} \left[2.6693 \cdot 10^{-26} \cdot \left(\frac{10^5 \cdot \text{cm}}{\text{sec}}\right) \cdot \left(\frac{\text{gm}}{K}\right)^{0.5} \right]}{\frac{(MW_3 \cdot T)^{0.5}}{(\sigma_3)^2 \cdot \Omega \mu \left(\frac{T}{\epsilon_3}\right)} \left[2.6693 \cdot 10^{-26} \cdot \left(\frac{10^5 \cdot \text{cm}}{\text{sec}}\right) \cdot \left(\frac{\text{gm}}{K}\right)^{0.5} \right]} \right. \\ \left. \frac{1.116 \cdot (MW_4 \cdot T)^{0.5}}{(3.115 \cdot 10^{-8} \cdot \text{cm})^2 \cdot \Omega \mu \left(\frac{T}{514 \cdot K}\right)} \left[2.6693 \cdot 10^{-26} \cdot \left(\frac{10^5 \cdot \text{cm}}{\text{sec}}\right) \cdot \left(\frac{\text{gm}}{K}\right)^{0.5} \right] \right]$$

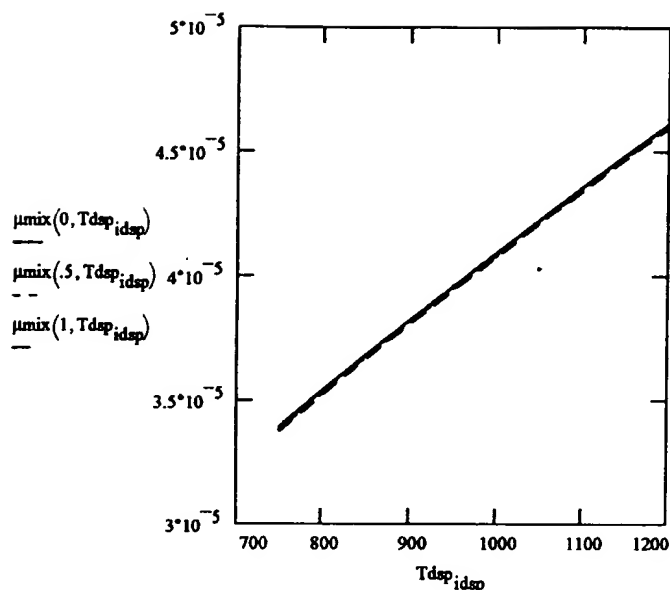
$$\mu(300 \cdot K) = \begin{bmatrix} 1.10281 \cdot 10^{-5} \\ 2.0603 \cdot 10^{-5} \\ 1.76981 \cdot 10^{-5} \\ 1.51851 \cdot 10^{-5} \\ 1.06784 \cdot 10^{-5} \end{bmatrix} \cdot \text{kg} \cdot \text{m}^{-1} \cdot \text{sec}^{-1}$$

$$\mu_{\text{mix}}(x, T) := \sum_{n=0}^4 \frac{y(\text{ych40}, x)_n \cdot \mu(T)_n}{\sum_{m=0}^4 y(\text{ych40}, x)_m \cdot \left[\frac{\left[1 + \left(\frac{\mu(T)_n}{\mu(T)_m}\right)^{0.5} \cdot \left(\frac{MW_m}{MW_n}\right)^{0.25} \right]^2}{\left[8 \cdot \left(1 + \frac{MW_n}{MW_m} \right) \right]^{0.5}} \right]}$$

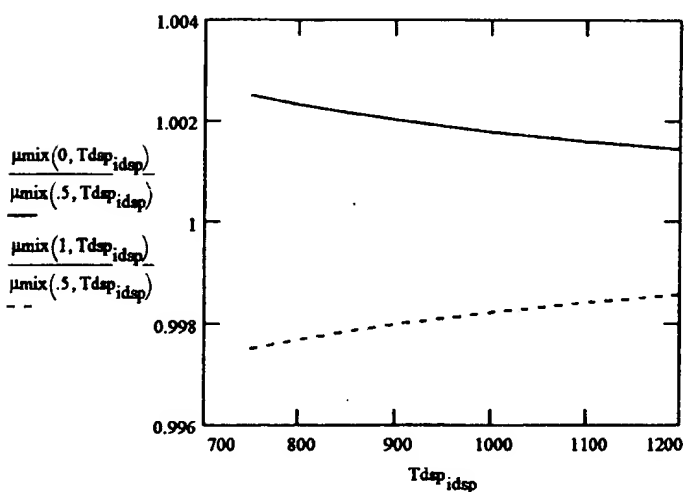
$$y(\text{ych40}, 0.5) = \begin{bmatrix} 0.00592 \\ 0.19074 \\ 0.76583 \\ 0.00592 \\ 0.03159 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$$\mu_{\text{mix}}(0.5, 300 \cdot K) = 0.00002 \cdot \text{kg} \cdot \text{m}^{-1} \cdot \text{sec}^{-1}$$

$$\text{ych40} = 0.01183$$



The viscosity of the CH₄ - air mixtures vary little with composition (< 0.5%), again because the fuel is so dilute. We can therefore neglect the effect of composition by choosing $x=0.5$ in all cases.



$T_{\text{dsp_idsp}}$	$\mu_{\text{mix}}(0.5, T_{\text{dsp_idsp}})$
$7.5 \cdot 10^2 \cdot \text{K}$	$3.38338 \cdot 10^{-5} \cdot \text{kg} \cdot \text{m}^{-1} \cdot \text{sec}^{-1}$
$8 \cdot 10^2 \cdot \text{K}$	$3.53056 \cdot 10^{-5} \cdot \text{kg} \cdot \text{m}^{-1} \cdot \text{sec}^{-1}$
$8.5 \cdot 10^2 \cdot \text{K}$	$3.67429 \cdot 10^{-5} \cdot \text{kg} \cdot \text{m}^{-1} \cdot \text{sec}^{-1}$
$9 \cdot 10^2 \cdot \text{K}$	$3.81491 \cdot 10^{-5} \cdot \text{kg} \cdot \text{m}^{-1} \cdot \text{sec}^{-1}$
$9.5 \cdot 10^2 \cdot \text{K}$	$3.95267 \cdot 10^{-5} \cdot \text{kg} \cdot \text{m}^{-1} \cdot \text{sec}^{-1}$
$1 \cdot 10^3 \cdot \text{K}$	$4.08779 \cdot 10^{-5} \cdot \text{kg} \cdot \text{m}^{-1} \cdot \text{sec}^{-1}$
$1.05 \cdot 10^3 \cdot \text{K}$	$4.22047 \cdot 10^{-5} \cdot \text{kg} \cdot \text{m}^{-1} \cdot \text{sec}^{-1}$
$1.1 \cdot 10^3 \cdot \text{K}$	$4.35088 \cdot 10^{-5} \cdot \text{kg} \cdot \text{m}^{-1} \cdot \text{sec}^{-1}$
$1.15 \cdot 10^3 \cdot \text{K}$	$4.47917 \cdot 10^{-5} \cdot \text{kg} \cdot \text{m}^{-1} \cdot \text{sec}^{-1}$
$1.2 \cdot 10^3 \cdot \text{K}$	$4.60547 \cdot 10^{-5} \cdot \text{kg} \cdot \text{m}^{-1} \cdot \text{sec}^{-1}$

$$\mu_{\text{mix}}(T) := \exp\left(-0.70216045 + 0.640874 \cdot \ln\left(\frac{T}{\text{K}}\right) + \frac{-14.24382 \cdot \text{K}}{T}\right) \cdot 10^{-6} \cdot \text{kg} \cdot \text{m}^{-1} \cdot \text{sec}^{-1}$$

$$\mu_{\text{mix}}(.5, 1000 \cdot \text{K}) = 4.08779 \cdot 10^{-5} \cdot \text{kg} \cdot \text{m}^{-1} \cdot \text{sec}^{-1}$$

$$\mu_{\text{mix}}(T(1000 \cdot \text{K})) = 4.08782 \cdot 10^{-5} \cdot \text{kg} \cdot \text{m}^{-1} \cdot \text{sec}^{-1}$$

Define thermal conductivity functions for light molecules

igas := 0, 1..4

CH4

O2

N2

CO2

H2O

$$a\lambda := \begin{bmatrix} -1.869 \\ -3.273 \\ 0.3919 \\ -7.215 \\ 7.341 \end{bmatrix} \quad b\lambda := \begin{bmatrix} 0.08727 \\ 0.09966 \\ 0.09816 \\ 0.08015 \\ -0.01013 \end{bmatrix} \quad c\lambda := \begin{bmatrix} 1.179 \cdot 10^{-4} \\ -(3.743 \cdot 10^{-5}) \\ -(5.067 \cdot 10^{-5}) \\ 5.477 \cdot 10^{-6} \\ 1.801 \cdot 10^{-4} \end{bmatrix} \quad d\lambda := \begin{bmatrix} -(3.614 \cdot 10^{-8}) \\ 9.732 \cdot 10^{-9} \\ 1.504 \cdot 10^{-8} \\ -(1.053 \cdot 10^{-8}) \\ -(9.1 \cdot 10^{-8}) \end{bmatrix}$$

$$\lambda(i, T) := \left[a\lambda_i + b\lambda_i \cdot \frac{T}{K} + c\lambda_i \cdot \left(\frac{T}{K} \right)^2 + d\lambda_i \cdot \left(\frac{T}{K} \right)^3 \right] \cdot 0.00001 \cdot \frac{W}{cm \cdot K}$$

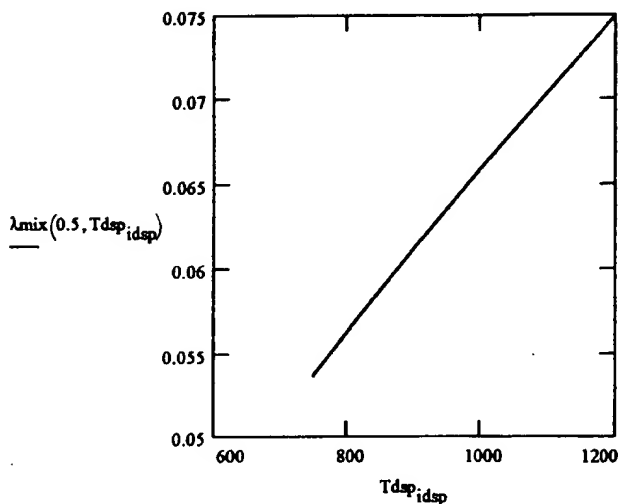
 $\lambda(\text{igas}, 1000 \cdot K)$

W/cm/K

$0.16716 \cdot \text{kg} \cdot \text{m} \cdot \text{sec}^{-3} \cdot \text{K}^{-1}$
$0.07163 \cdot \text{kg} \cdot \text{m} \cdot \text{sec}^{-3} \cdot \text{K}^{-1}$
$0.06292 \cdot \text{kg} \cdot \text{m} \cdot \text{sec}^{-3} \cdot \text{K}^{-1}$
$0.06788 \cdot \text{kg} \cdot \text{m} \cdot \text{sec}^{-3} \cdot \text{K}^{-1}$
$0.08631 \cdot \text{kg} \cdot \text{m} \cdot \text{sec}^{-3} \cdot \text{K}^{-1}$

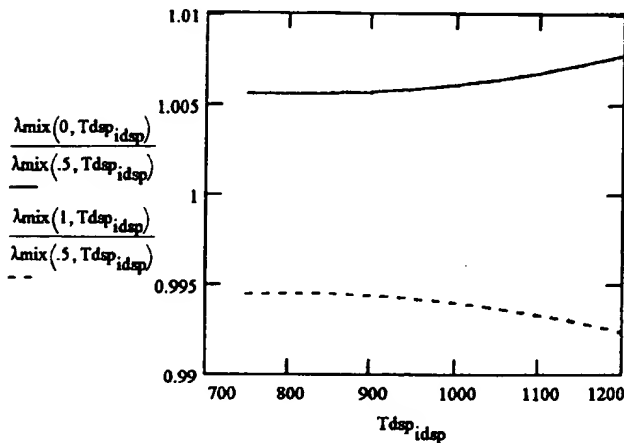
$$\lambda_{\text{mix}}(x, T) := \sum_{i=0}^4 \frac{y(\text{ych40}, x)_i \cdot \lambda(i, T)}{\sum_{j=0}^4 y(\text{ych40}, x)_j \cdot \left[\frac{1 + \left(\frac{\mu(T)_i}{\mu(T)_j} \right)^{0.5} \cdot \left(\frac{MW_j}{MW_i} \right)^{0.25} \right]^2 \cdot \left[8 \cdot \left(1 + \frac{MW_i}{MW_j} \right) \right]^{0.5}}$$

$$\lambda_{\text{mix}}(.0, 1000 \cdot K) = 0.00066 \cdot \frac{W}{cm \cdot K}$$

 $T_{\text{dsp_idsp}}$ $\lambda_{\text{mix}}(0.5, T_{\text{dsp_idsp}})$

$7.5 \cdot 10^2 \cdot K$
$8 \cdot 10^2 \cdot K$
$8.5 \cdot 10^2 \cdot K$
$9 \cdot 10^2 \cdot K$
$9.5 \cdot 10^2 \cdot K$
$1 \cdot 10^3 \cdot K$
$1.05 \cdot 10^3 \cdot K$
$1.1 \cdot 10^3 \cdot K$
$1.15 \cdot 10^3 \cdot K$
$1.2 \cdot 10^3 \cdot K$

$0.05362 \cdot \text{kg} \cdot \text{m} \cdot \text{sec}^{-3} \cdot \text{K}^{-1}$
$0.05621 \cdot \text{kg} \cdot \text{m} \cdot \text{sec}^{-3} \cdot \text{K}^{-1}$
$0.05872 \cdot \text{kg} \cdot \text{m} \cdot \text{sec}^{-3} \cdot \text{K}^{-1}$
$0.06117 \cdot \text{kg} \cdot \text{m} \cdot \text{sec}^{-3} \cdot \text{K}^{-1}$
$0.06355 \cdot \text{kg} \cdot \text{m} \cdot \text{sec}^{-3} \cdot \text{K}^{-1}$
$0.06589 \cdot \text{kg} \cdot \text{m} \cdot \text{sec}^{-3} \cdot \text{K}^{-1}$
$0.06818 \cdot \text{kg} \cdot \text{m} \cdot \text{sec}^{-3} \cdot \text{K}^{-1}$
$0.07043 \cdot \text{kg} \cdot \text{m} \cdot \text{sec}^{-3} \cdot \text{K}^{-1}$
$0.07266 \cdot \text{kg} \cdot \text{m} \cdot \text{sec}^{-3} \cdot \text{K}^{-1}$
$0.07488 \cdot \text{kg} \cdot \text{m} \cdot \text{sec}^{-3} \cdot \text{K}^{-1}$



The thermal conductivity varies > 1% with conversion. Selection of 50% conversion gives an error range of +.5-.5% at 1000K. This is likely to be smaller than the accuracy of measured thermal conductivity. Therefore we again define a composition independent formula to increase speed in calculating derived transport properties

$$\lambda_{\text{mix}}T(T) := \exp\left(-7.073383 + 0.6397005 \cdot \ln\left(\frac{T}{K}\right) + \frac{-65.2387 \cdot K}{T}\right) \cdot W \cdot m^{-1} \cdot K^{-1}$$

$$\lambda_{\text{mix}}(.5, 1000 \cdot K) = 0.06589 \cdot m^{-1} \cdot K^{-1} \cdot W$$

$$\lambda_{\text{mix}}T(1000 \cdot K) = 0.06589 \cdot m^{-1} \cdot K^{-1} \cdot W$$

Determine the heat capacity and enthalpy functions of the fuel-air mixtures for the evaluation of temperature rise

Define heat capacities and heat of combustion:

$$Cp_{\text{coef}} := \begin{bmatrix} 19.25 & .05213 & 0.00001197 & -0.00000001132 \\ 28.11 & -0.000368 & 0.00001746 & -0.00000001065 \\ 31.15 & -0.01357 & 0.0000268 & -0.00000001168 \\ 19.8 & 0.07344 & -0.00005602 & 0.00000001715 \\ 32.24 & 0.001924 & 0.00001055 & -0.000000003596 \\ -9.52 & 0.5066 & -0.0002729 & 0.00000005723 \\ -76.19 & 0.7867 & -0.0004204 & 0.00000007516 \\ -37.18 & 0.8122 & -0.0004509 & 0.00000009705 \end{bmatrix}$$

$$Cp(\text{igas}, T) := \sum_{jj=0}^3 Cp_{\text{coef}}_{\text{igas}, jj} \cdot \left(\frac{T}{K}\right)^{jj} \cdot \frac{J}{K}$$

J/mol/K

$$Cp(0, 300 \cdot K) = 35.66066 \cdot K^{-1} \cdot J$$

$$Cp(5, 300 \cdot K) = 119.44421 \cdot K^{-1} \cdot J$$

$$Cp(6, 300 \cdot K) = 124.01332 \cdot K^{-1} \cdot J$$

$$Cp(7, 300 \cdot K) = 168.51935 \cdot K^{-1} \cdot J$$

$$y(\text{ych40}, 0.5) = \begin{bmatrix} 0.00592 \\ 0.19074 \\ 0.76583 \\ 0.00592 \\ 0.03159 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$$Cp_{\text{mix}}(x, T) := \sum_{jk=0}^4 Cp(jk, T) \cdot y(\text{ych40}, x)_{jk}$$

$$Cp_{\text{mix}}(0.5, 998 \cdot K) = 33.66993 \cdot J \cdot K^{-1}$$

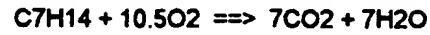
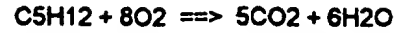
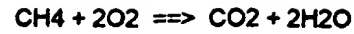
Define heats of combustion

$$\Delta C_{pcomb}(T) := (C_p(3, T) + 2 \cdot C_p(4, T)) - (C_p(0, T) + 2 \cdot C_p(1, T))$$

$$\Delta C_{pcomb5}(T) := (5 \cdot C_p(3, T) + 6 \cdot C_p(4, T)) - (C_p(5, T) + 8 \cdot C_p(1, T))$$

$$\Delta C_{pcomb7}(T) := (7 \cdot C_p(3, T) + 7 \cdot C_p(4, T)) - (C_p(6, T) + 10.5 \cdot C_p(1, T))$$

$$\Delta C_{pcomb9}(T) := (9 \cdot C_p(3, T) + 9 \cdot C_p(4, T)) - (C_p(7, T) + 13.5 \cdot C_p(1, T))$$



$$\Delta H_f := \begin{bmatrix} -74900 \cdot J \\ 0 \cdot J \\ 0 \cdot J \\ -393800 \cdot J \\ -242000 \cdot J \\ -154600 \cdot J \\ -119400 \cdot J \\ -103600 \cdot J \end{bmatrix}$$

$$\Delta C_{pcomb}(298 \cdot K) = 10.38812 \cdot K^{-1} \cdot J$$

$$\frac{\Delta C_{pcomb7}(298 \cdot K)}{7} = 9.35823 \cdot K^{-1} \cdot J$$

$$\frac{\Delta C_{pcomb5}(298 \cdot K)}{5} = 6.97449 \cdot kg \cdot m^2 \cdot sec^{-2} \cdot K^{-1}$$

$$\frac{\Delta C_{pcomb9}(298 \cdot K)}{9} = 8.3177 \cdot K^{-1} \cdot J$$

Define enthalpy function for individual components and ΔH for fuels:

$$H_f(nm, T) := \Delta H_{f_m} + \int_{298 \cdot K}^T C_p(nm, T_x) dT_x$$

$$\Delta H_{comb}(T) := \left[(\Delta H_{f_3} + 2 \cdot \Delta H_{f_4}) - (\Delta H_{f_0} + 2 \cdot \Delta H_{f_1}) \right] + \int_{298 \cdot K}^T \Delta C_{pcomb}(T_x) dT_x$$

$$\Delta H_{comb5}(T) := \left[(5 \cdot \Delta H_{f_3} + 6 \cdot \Delta H_{f_4}) - (\Delta H_{f_0} + 8 \cdot \Delta H_{f_1}) \right] + \int_{298 \cdot K}^T \Delta C_{pcomb5}(T_x) dT_x$$

$$\Delta H_{comb7}(T) := \left[(7 \cdot \Delta H_{f_3} + 7 \cdot \Delta H_{f_4}) - (\Delta H_{f_0} + 10.5 \cdot \Delta H_{f_1}) \right] + \int_{298 \cdot K}^T \Delta C_{pcomb7}(T_x) dT_x$$

$$\Delta H_{comb9}(T) := \left[(9 \cdot \Delta H_{f_3} + 9 \cdot \Delta H_{f_4}) - (\Delta H_{f_0} + 13.5 \cdot \Delta H_{f_1}) \right] + \int_{298 \cdot K}^T \Delta C_{pcomb9}(T_x) dT_x$$

$H_f(\text{igas}, 1000 \cdot K)$

-36559.44819 · kg · m ² · sec ⁻²
22590.03871 · kg · m ² · sec ⁻²
21484.78794 · kg · m ² · sec ⁻²
-3.60367 · 10 ⁵ · kg · m ² · sec ⁻²
-2.15959 · 10 ⁵ · kg · m ² · sec ⁻²

Evaluate a few values of ΔH for CH_4 , C_5H_{12} , C_7H_{14} , and C_9H_{18} :

$$\Delta H_{comb}(800 \cdot K) = -8.00306 \cdot 10^5 \cdot J \quad \frac{\Delta H_{comb5}(800 \cdot K)}{5} = -6.69221 \cdot 10^5 \cdot J$$

$$\frac{\Delta H_{comb7}(800 \cdot K)}{7} = -6.2472 \cdot 10^5 \cdot J \quad \frac{\Delta H_{comb9}(800 \cdot K)}{9} = -6.26002 \cdot 10^5 \cdot J$$

Define the mixture enthalpies and determine the fuel composition needed for 511F temperature rise from 1000F.

igas := 0, 1..7

$$H_{mix}(x, T) := \sum_{k_{gas}=0}^7 y(y_{ch40}, x)_{k_{gas}} \cdot H_f(k_{gas}, T) \quad y_{ch40} = 0.01183$$

$$H_{mix}(0, 810.93 \cdot K) = 1.006514 \cdot 10^4 \cdot J \quad H_{mix}(1, 1094.82 \cdot K) = 1.006518 \cdot 10^4 \cdot J$$

Determines CH4 inlet concentration

$$H_{mix5}(x, T) := \sum_{k_{gas}=0}^7 y5(y_{0c5h12}, x)_{k_{gas}} \cdot H_f(k_{gas}, T) \quad y_{0c5h12} := 0.0028968$$

Determines C5H12 inlet concentration

$$H_{mix5}(0, 810.93 \cdot K) = 1.058499 \cdot 10^4 \cdot J \quad H_{mix5}(1, 1094.82 \cdot K) = 1.058492 \cdot 10^4 \cdot J$$

$$H_{mix7}(x, T) := \sum_{k_{gas}=0}^7 y7(y_{0c7h14}, x)_{k_{gas}} \cdot H_f(k_{gas}, T) \quad y_{0c7h14} := 0.0021859$$

Determines C7H14 inlet concentration

$$H_{mix7}(0, 810.93 \cdot K) = 1.075807 \cdot 10^4 \cdot J \quad H_{mix7}(1, 1094.82 \cdot K) = 1.075812 \cdot 10^4 \cdot J$$

$$H_{mix9}(x, T) := \sum_{k_{gas}=0}^7 y9(y_{0c9h18}, x)_{k_{gas}} \cdot H_f(k_{gas}, T) \quad y_{0c9h18} := 0.0016878$$

Determines C9H18 inlet concentration

$$H_{mix9}(0, 810.93 \cdot K) = 1.083024 \cdot 10^4 \cdot J \quad H_{mix9}(1, 1094.82 \cdot K) = 1.083028 \cdot 10^4 \cdot J$$

Define momentum and thermal diffusivities:

$$P = 3.039 \cdot 10^5 \cdot \text{Pa}$$

$$\alpha(\text{igas}, T) := \frac{\lambda(\text{igas}, T) \cdot R \cdot T}{C_p(\text{igas}, T) \cdot P}$$

$$\alpha(0, 300 \cdot \text{K}) = 0.07813 \cdot \text{sec}^{-1} \cdot \text{cm}^2$$

$$\alpha_{\text{mix}}(x, T) := \frac{\lambda_{\text{mix}}(x, T) \cdot R \cdot T}{C_{p_{\text{mix}}}(x, T) \cdot P}$$

$$\alpha_{\text{mix}}(.5, 1000 \cdot \text{K}) = 0.5352 \cdot \text{sec}^{-1} \cdot \text{cm}^2$$

$$\nu_{\text{mix}}(x, T) := \frac{\mu_{\text{mix}}(x, T)}{\rho_{\text{mix}}(x, T)}$$

$$\rho_{\text{mix}}(.5, 1000 \cdot \text{K}) = 1.04117 \cdot 10^{-3} \cdot \text{gm} \cdot \text{cm}^{-3}$$

$$\nu_{\text{mix}}(.5, 1000 \cdot \text{K}) = 0.3926 \cdot \text{sec}^{-1} \cdot \text{cm}^2$$

$$D_{\text{ch4}}(.5, 1000 \cdot \text{K}) = 0.5855 \cdot \text{sec}^{-1} \cdot \text{cm}^2$$

$$D_{\text{c5h12}}(.5, 1000 \cdot \text{K}) = 0.1957 \cdot \text{sec}^{-1} \cdot \text{cm}^2$$

$$D_{\text{c7h14}}(0.5, 1000 \cdot \text{K}) = 0.1698 \cdot \text{sec}^{-1} \cdot \text{cm}^2$$

$$D_{\text{c9h18}}(.5, 1000 \cdot \text{K}) = 0.13431 \cdot \text{sec}^{-1} \cdot \text{cm}^2$$

Define Prandtl, Schmidt, and Lewis numbers

$$\text{Pr}(x, T) := \frac{\nu_{\text{mix}}(x, T)}{\alpha_{\text{mix}}(x, T)}$$

$$\text{Pr}(.5, 1000 \cdot \text{K}) = 0.73359$$

$$\text{Sc}(x, T) := \frac{\nu_{\text{mix}}(x, T)}{D_{\text{ch4}}(x, T)}$$

$$\text{Sc}(.5, 1000 \cdot \text{K}) = 0.67054$$

$$\text{Sc5}(x, T) := \frac{\nu_{\text{mix}}(x, T)}{D_{\text{c5h12}}(x, T)}$$

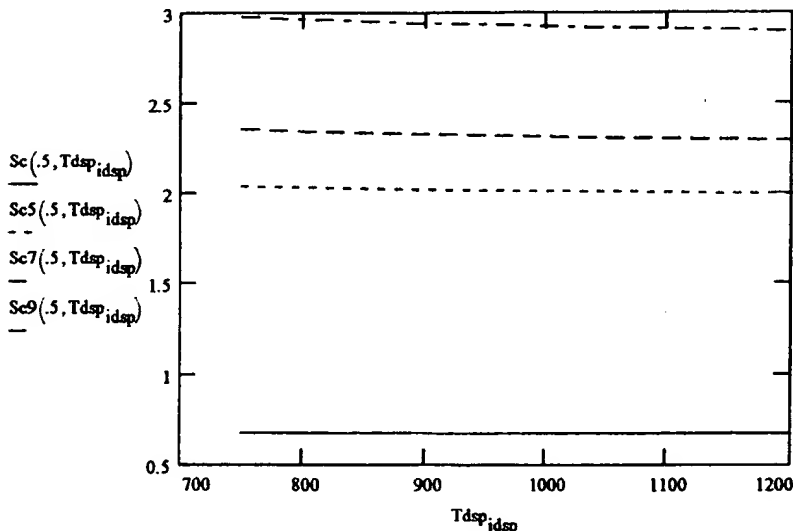
$$\text{Sc5}(.5, 1000 \cdot \text{K}) = 2.00639$$

$$\text{Sc7}(x, T) := \frac{\nu_{\text{mix}}(x, T)}{D_{\text{c7h14}}(x, T)}$$

$$\text{Sc7}(.5, 1000 \cdot \text{K}) = 2.31224$$

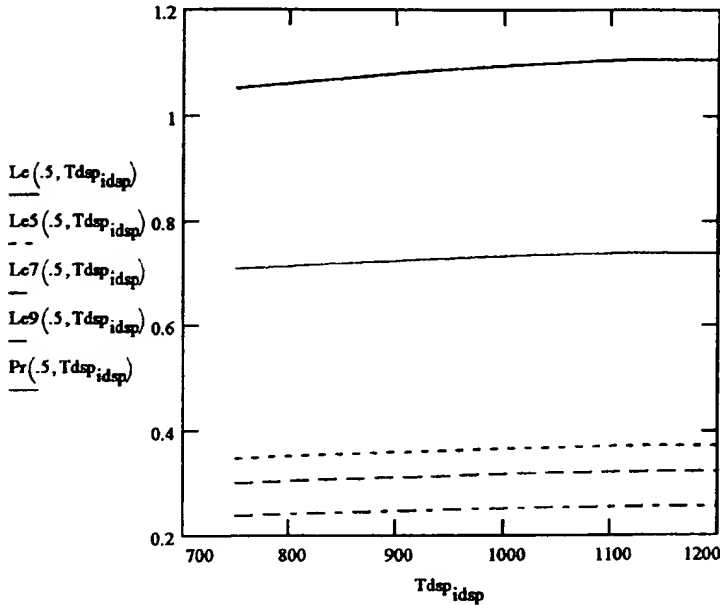
$$\text{Sc9}(x, T) := \frac{\nu_{\text{mix}}(x, T)}{D_{\text{c9h18}}(x, T)}$$

$$\text{Sc9}(.5, 1000 \cdot \text{K}) = 2.92325$$



These relations have weak temperature dependence and (presumably) very weak dependence on composition

$$\begin{aligned} Le(x, T) &:= \frac{D_{ch4}(x, T)}{\alpha_{mix}(x, T)} & Le(.5, 1000 \cdot K) &= 1.09404 & Le5(x, T) &:= \frac{D_{c5h12}(x, T)}{\alpha_{mix}(x, T)} & Le5(.5, 1000 \cdot K) &= 0.36563 \\ Le7(x, T) &:= \frac{D_{c7h14}(x, T)}{\alpha_{mix}(x, T)} & Le7(.5, 1000 \cdot K) &= 0.31726 & Le9(x, T) &:= \frac{D_{c9h18}(x, T)}{\alpha_{mix}(x, T)} & Le9(.5, 1000 \cdot K) &= 0.25095 \end{aligned}$$



The Lewis numbers show approximately the temperature rise at the wall of an active catalyst relative to the adiabatic temperature rise at that point.

Clearly temperature (and composition) have little influence on the ΔT at the wall, while the nature of the fuel molecule has a strong effect (from $0.25 \cdot \Delta T_{adiab}$ for C9 to $1.1 \cdot \Delta T_{adiab}$ for CH4)

Can remove compositional dependence for most property functions

$$\rho_{mixT}(T) := MW_{mix}(0.5) \cdot \frac{P}{R \cdot T}$$

$$\nu_{mixT}(T) := \frac{\mu_{mixT}(T)}{\rho_{mixT}(T)}$$

$$ScT(T) := \frac{\mu_{mixT}(T)}{D_{ch4T}(T) \cdot \rho_{mix}(0.5, T)}$$

$$Sc7T(T) := \frac{\mu_{mixT}(T)}{D_{c7h14T}(T) \cdot \rho_{mix}(0.5, T)}$$

These functions speed calculations of Nu numbers and heat and mass transfer coefficients

This ends the extended section that defines gas properties for the combustion of several fuel air mixtures.

CHPSTONE.MCU

Define honeycomb configurations

Diao := 9-in Diao = 22.86-cm Diai := 4-in Diai = 10.16-cm Lhc := 3.5-in Lhc = 8.89-cm

With bypass change Diao to 8.5 in Bypass := 0 Bypass - 0, 0.2, 0.4 Lhc - 3.5, 4 in

Honeycombs: Represent as square channel metal alloy wall 0.05 mm, uncoated

Cells1 := 100-in² dwall1 := 0.009-cm Cells2 := 200-in² dwall2 := 0.009-cm

dcell1 := (Cells1)^{-0.5} - dwall1

dcell2 := (Cells2)^{-0.5} - dwall2

Describe 100 and 200 cpi dimensions, although not expected to be used

dcell1 = 0.245-cm

ks1 := 0.002-cm

dcell2 = 0.17061-cm

ks2 := 0.002-cm

scell1 := dcell1² · Cells1

scell1 = 0.93039

scell2 := dcell2² · Cells2

scell2 = 0.90229

Cells4 := 400-in²

dwall4 := 0.007-cm

Cells6 := 600-in²

dwall6 := 0.007-cm

dcell4 := (Cells4)^{-0.5} - dwall4

dcell4 = 0.12-cm

dcell6 := (Cells6)^{-0.5} - dwall6

dcell6 = 0.0967-cm

dcell4 = 0.12-cm

ks4 := 0.001-cm

dcell6 = 0.0967-cm

ks6 := 0.001-cm

scell4 := dcell4² · Cells4

scell4 = 0.8928

scell6 := dcell6² · Cells6

scell6 = 0.86955

Packed Beds: Cylindrical (conical) geometry

Dinr := 6-in

Doutr := 7-in

Wbed := 7-in

Lbed := 0.75-in

Dinr = 15.24-cm

Doutr = 17.78-cm

Wbed = 17.78-cm

Smono := $\frac{\pi}{4} \cdot (Diao^2 - Diai^2)$

Sbed := $\pi \cdot \left(\frac{Dinr + Doutr}{2} \right) \cdot Wbed$

$\frac{Smono}{Sbed} = 0.35714$

Define initial combustion conditions

Adjust U0 to fit U(Tin)=7 m/sec w/o bypass flow

Uref := 7 $\frac{m}{sec}$

Tin := (537.778 + 273.15) · K

Tin = 810.928 · K

P = 3.039 · 10⁵ · kg · m⁻¹ · sec⁻²

M0 := Uref · $\rho_{mix}(0, Tin) \cdot \left[\frac{\pi}{4} \cdot ((9-in)^2 - (4-in)^2) \right]$

M0 = 0.29601 · kg · sec⁻¹

Tout := (821.667 + 273.15) · K

U0 := $\frac{M0 \cdot (1 - Bypass)}{\rho_{mix}(0, Tin) \cdot \frac{\pi}{4} \cdot (Diao^2 - Diai^2)}$

Tout = 1094.817 · K

U(T) := U0 · $\frac{T}{Tin}$

U(Tin) = 7 · m · sec⁻¹

G0 := U(Tin) · $\rho_{mix}(0, Tin)$

Ubed(T) := $\frac{M0}{\rho_{mix}(0, Tin) \cdot Sbed}$

Ubed(Tin) = 2.5 · m · sec⁻¹

G0 = 8.98749 · kg · m⁻² · sec⁻¹

Evaluate Reynolds numbers for use in calculating the momentum, heat, and mass transfer functions:

$$\text{Rehc4}(T) := \frac{G0 \cdot d_{\text{cell4}}}{s_{\text{cell4}} \cdot \mu_{\text{mix}}(T)} \quad \text{Rehc4}(T_{\text{in}}) = 339.11451$$

$$\text{Rehc6}(T) := \frac{G0 \cdot d_{\text{cell6}}}{s_{\text{cell6}} \cdot \mu_{\text{mix}}(T)} \quad \text{Rehc6}(T_{\text{in}}) = 280.56407$$

For laminar flow with entrance effect (adapted from Kays & Crawford, "Convective Heat and Mass Transfer"):

$$\text{cfric4}(T, z) := \frac{14.227}{\text{Rehc4}(T)} \left[1 + 0.046263 \cdot \left(\text{Rehc4}(T) \cdot \frac{d_{\text{cell4}}}{z} \right)^{0.45363} \right]$$

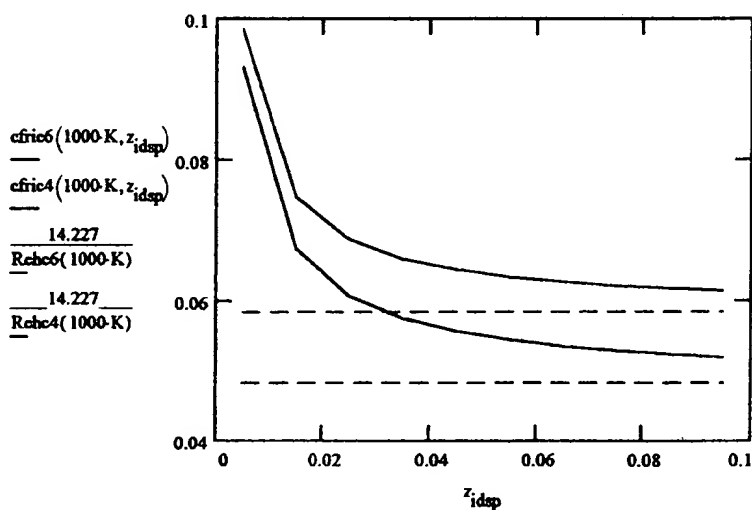
$$\text{cfric6}(T, z) := \frac{14.227}{\text{Rehc6}(T)} \left[1 + 0.046263 \cdot \left(\text{Rehc6}(T) \cdot \frac{d_{\text{cell6}}}{z} \right)^{0.45363} \right]$$

Average coefficient of friction

Calculate monolith pressure drop in several monoliths with entrance effect:

$$z_{\text{idsp}} := 0.5 \cdot \text{cm} + 1 \cdot \text{idsp} \cdot \text{cm}$$

$$U_{\text{dsp}} := (4 + \text{idsp}) \cdot \text{m} \cdot \text{sec}^{-1}$$



The entrance effect for ΔP of a channel in laminar flow is significant even to 3.5 in. length.

04PSTONE.MCD

$$T_{avg} := \frac{T_{in} + T_{out}}{2}$$

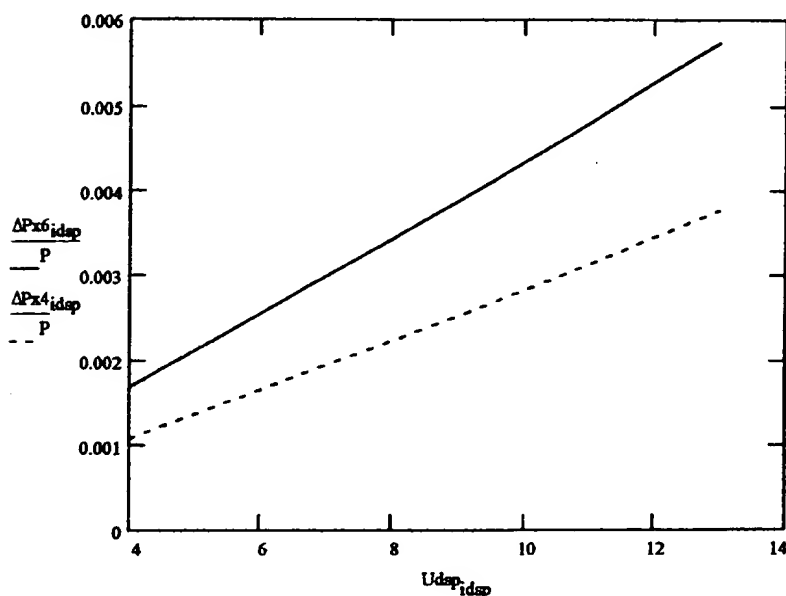
$$c_{f,ix}(x,z) := \frac{14.227}{x} \cdot (1 + 0.0462363 \cdot (x \cdot z))^{0.45363}$$

$$R_{ex6_idsp} := \frac{d_{cell6}}{s_{cell6}} \cdot \frac{U_{dsp_idsp}}{v_{mixT}(T_{avg})}$$

$$R_{ex4_idsp} := \frac{d_{cell4}}{s_{cell4}} \cdot \frac{U_{dsp_idsp}}{v_{mixT}(T_{avg})}$$

$$\Delta P_{x4_idsp} := 4 \cdot c_{f,ix} \left(R_{ex4_idsp}, \frac{d_{cell4}}{L_{hc}} \right) \cdot \frac{\rho_{mixT}(T_{avg})}{2} \cdot \left(\frac{U_{dsp_idsp}}{s_{cell4}} \right)^2 \cdot \frac{L_{hc}}{d_{cell4}}$$

$$\Delta P_{x6_idsp} := 4 \cdot c_{f,ix} \left(R_{ex6_idsp}, \frac{d_{cell6}}{L_{hc}} \right) \cdot \frac{\rho_{mixT}(T_{avg})}{2} \cdot \left(\frac{U_{dsp_idsp}}{s_{cell6}} \right)^2 \cdot \frac{L_{hc}}{d_{cell6}}$$



$\Delta P/P < 0.5\%$ to about 11 m/sec

$$\Delta P_{hc6}(T) := 4 \cdot c_{f,ic6}(T, L_{hc}) \cdot \frac{\rho_{mixT}(T) \cdot \left(\frac{U(T)}{s_{cell6}} \right)^2}{2} \cdot \frac{L_{hc}}{d_{cell6}}$$

$$T_{avg} = 952.8725 \cdot K$$

$$U(T_{avg}) = 8.22528 \cdot m \cdot sec^{-1}$$

$$\frac{\Delta P_{hc6}(T_{in})}{P} = 0.00271$$

$$\frac{\Delta P_{hc6}(T_{out})}{P} = 0.00441$$

$$\frac{\Delta P_{hc6}(T_{avg})}{P} = 0.00352$$

$$\Delta P_{hc4}(T) := 4 \cdot c_{f,ic4}(T, L_{hc}) \cdot \frac{\rho_{mixT}(T) \cdot \left(\frac{U(T)}{s_{cell4}} \right)^2}{2} \cdot \frac{L_{hc}}{d_{cell4}}$$

$$\frac{\Delta P_{hc4}(T_{avg})}{P} = 0.00228$$

Find 1-D heat and mass transfer rates via Nusselt formulas

Averaged Nu for 600 cpi square channels (fully developed laminar flow) taken from Rosner:

$$\text{NuhavgR6}(z) := 2.976 \cdot \left[1 + \left(\frac{7.6 \cdot z}{\text{Rehc6}(\text{Tavg}) \cdot \text{Pr}(.5, \text{Tavg}) \cdot \text{dccl6}} \right)^{\frac{1}{3}} \right]^{\frac{8}{3}}$$

$$\frac{7.6 \cdot (2 \cdot \text{cm})}{\text{Rehc6}(\text{Tavg}) \cdot \text{Pr}(.5, \text{Tavg}) \cdot \text{dccl6}} = 0.85369$$

$$\text{NuhavgR6}(\text{Lhc}) = 2.98649$$

$$\text{NumavgR6}(z) := 2.976 \cdot \left[1 + \left(\frac{7.6 \cdot z}{\text{Rehc6}(\text{Tavg}) \cdot \text{ScT}(\text{Tavg}) \cdot \text{dccl6}} \right)^{\frac{1}{3}} \right]^{\frac{8}{3}}$$

$$\text{NumavgR6}(\text{Lhc}) = 2.98441$$

$$\text{Num5avgR6}(z) := 2.976 \cdot \left[1 + \left(\frac{7.6 \cdot z}{\text{Rehc6}(\text{Tavg}) \cdot \text{Sc5}(.5, \text{Tavg}) \cdot \text{dccl6}} \right)^{\frac{1}{3}} \right]^{\frac{8}{3}}$$

$$\text{Num5avgR6}(\text{Lhc}) = 3.11102$$

$$\text{Num7avgR6}(z) := 2.976 \cdot \left[1 + \left(\frac{7.6 \cdot z}{\text{Rehc6}(\text{Tavg}) \cdot \text{Sc7T}(\text{Tavg}) \cdot \text{dccl6}} \right)^{\frac{1}{3}} \right]^{\frac{8}{3}}$$

$$\text{Num7avgR6}(\text{Lhc}) = 3.16167$$

$$\text{Num7avgR4}(z) := 2.976 \cdot \left[1 + \left(\frac{7.6 \cdot z}{\text{Rehc4}(\text{Tavg}) \cdot \text{Sc7T}(\text{Tavg}) \cdot \text{dccl4}} \right)^{\frac{1}{3}} \right]^{\frac{8}{3}}$$

$$\text{Num7avgR4}(\text{Lhc}) = 3.3902$$

$$\text{Num9avgR6}(z) := 2.976 \cdot \left[1 + \left(\frac{7.6 \cdot z}{\text{Rehc6}(\text{Tavg}) \cdot \text{Sc9}(.5, \text{Tavg}) \cdot \text{dccl6}} \right)^{\frac{1}{3}} \right]^{\frac{8}{3}}$$

$$\text{Num9avgR6}(\text{Lhc}) = 3.2775$$

The Nusselt numbers for mass transfer show small (< 5%) compensation for the low diffusivity of the higher hydrocarbons.

Use exponential functions implied by the definition of average (integrated) Num functions to calculate exit mole fractions.

$$y_{c7h14}(T, z) := y_{0c7h14} \cdot \exp\left(\frac{-4 \cdot z \cdot \text{Num7avgR6}(z)}{\text{Rehc6}(T) \cdot \text{ScT}(T) \cdot \text{dcell6}}\right)$$

$$\frac{y_{c7h14}(\text{Tavg}, \text{Lhc})}{y_{0c7h14}} = 0.13705$$

$$y_{ch4}(T, z) := y_{ch40} \cdot \exp\left(\frac{-4 \cdot z \cdot \text{NumavgR6}(z)}{\text{Rehc6}(T) \cdot \text{ScT}(T) \cdot \text{dcell6}}\right)$$

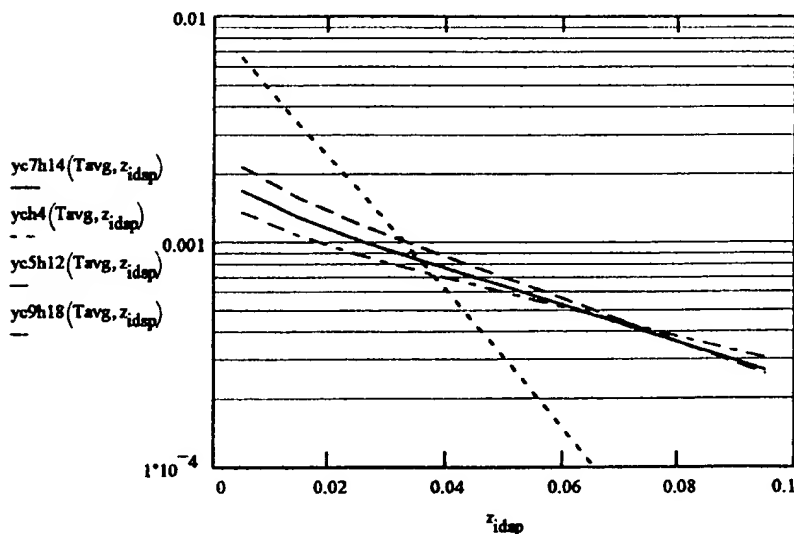
$$\frac{y_{ch4}(\text{Tavg}, \text{Lhc})}{y_{ch40}} = 0.001533$$

$$y_{c5h12}(T, z) := y_{0c5h12} \cdot \exp\left(\frac{-4 \cdot z \cdot \text{Num7avgR6}(z)}{\text{Rehc6}(T) \cdot \text{Sc5}(0.5, T) \cdot \text{dcell6}}\right)$$

$$\frac{y_{c5h12}(\text{Tavg}, \text{Lhc})}{y_{0c5h12}} = 0.10114$$

$$y_{c9h18}(T, z) := y_{0c9h18} \cdot \exp\left(\frac{-4 \cdot z \cdot \text{Num9avgR6}(z)}{\text{Rehc6}(T) \cdot \text{Sc9}(0.5, T) \cdot \text{dcell6}}\right)$$

$$\frac{y_{c9h18}(\text{Tavg}, \text{Lhc})}{y_{0c9h18}} = 0.19604$$



$$z_g = 0.095 \cdot \text{m}$$

$$z_g = 3.74016 \cdot \text{in}$$

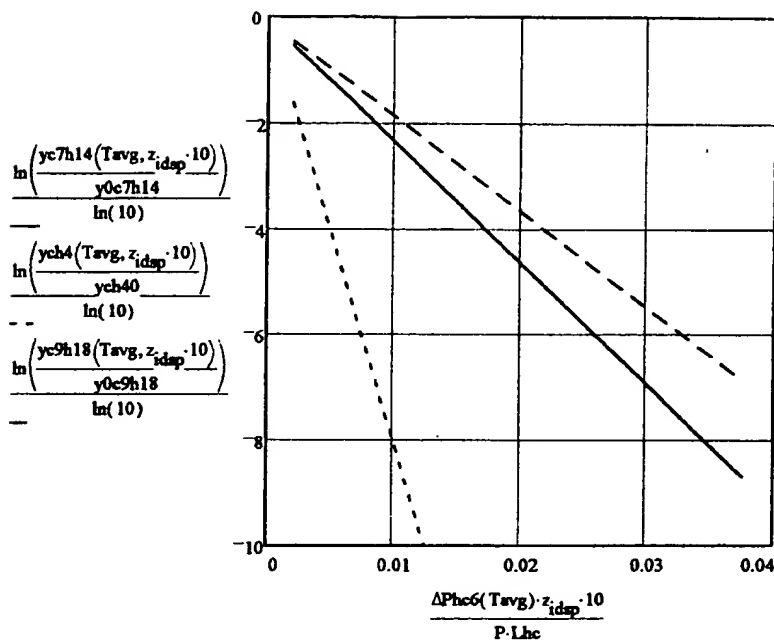
Summary if 600 cpi Metal Monolith Performance

%Bypass	Length(in)	Diao(in)	Yout/Yin C7H14	Yout/Yin CH4	ΔP/P
0	3.5	9.0	0.13705	0.001533	0.00352
0	4	9.0	0.10679	0.000611	0.00400
20	3.5	8.5	0.11888	0.000906	0.00324
20	4	8.5	0.09055	0.000335	0.00368
40	3.5	8.5	0.06266	0.000089	0.00240
40	4	8.5	0.04317	0.000023	0.00273

Bypass = 0
Lhc = 3.5 in
Diao = 9 in

These values are conservative and do not account for the higher average temperature with the higher F/A ratios and do not account for hydrothermal entry.

CAPSTONE MOD



Constant Flow 8.2 m/sec
Variable Length to 89 cm

$$U(T_{avg}) = 8.22528 \cdot m \cdot sec^{-1}$$

$$10 \cdot L_{hc} = 88.9 \cdot cm$$

Conversions at $\Delta P/P = 0.01$

$$CH_4 = 1.06 \cdot 10^{-8}$$

$$C_7H_{14} = 4.8 \cdot 10^{-3}$$

$$C_9H_{18} = 1.44 \cdot 10^{-2}$$

$$z = 25.25 \cdot cm$$

Conversions at $\Delta P/P = 0.02$

$$CH_4 = 1.14 \cdot 10^{-16}$$

$$C_7H_{14} = 2.41 \cdot 10^{-5}$$

$$C_9H_{18} = 2.21 \cdot 10^{-4}$$

$$z = 50.5 \cdot cm$$

$$z_x = 25.25 \cdot cm$$

$$\frac{\Delta P/P}{P \cdot L_{hc}} = 0.01000$$

$$\frac{y_{C7H14}(T_{avg}, z_x)}{y_{0C7H14}} = 4.80371 \cdot 10^{-3}$$

$$\frac{y_{C4H10}(T_{avg}, z_x)}{y_{0C4H10}} = 1.06492 \cdot 10^{-8}$$

$$\frac{y_{C9H18}(T_{avg}, z_x)}{y_{0C9H18}} = 1.44218 \cdot 10^{-2}$$

The 600 cpi monolith has low pressure drop at 8.89 cm length. If it's length were extended to give 1.0% and 2.0% fractional pressure drop, then C7H14 conversions would increase to 99.5% and 99.998% respectively

102280-EGEE60

Set up properties for CO to calculate the conversion of dilute CO and hydrocarbons downstream of the turbine

$$Dco1(x, T) := \frac{\frac{P}{Pref}}{\sum_{jgas=0}^7 \frac{y(ych40, x)_{jgas}}{Diff(8, jgas, T)}}$$

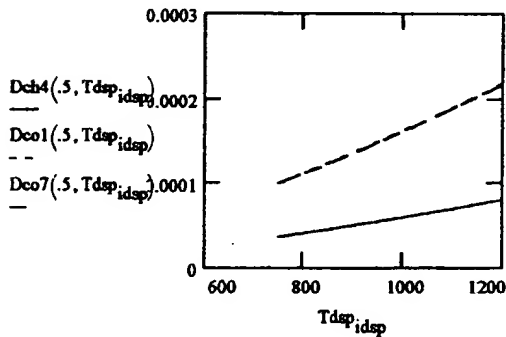
$$Dco1(.5, Tin) = 1.12854 \cdot \text{sec}^{-1} \cdot \text{cm}^2 \quad Pref = 1 \cdot \text{atm}$$

$$Dch4(.5, Tin) = 0.41195 \cdot \text{sec}^{-1} \cdot \text{cm}^2 \quad P = 3 \cdot \text{atm}$$

$$Dco7(x, T) := \frac{\frac{P}{Pref}}{\sum_{jgas=0}^7 \frac{y7(y0c7h14, x)_{jgas}}{Diff(8, jgas, T)}}$$

$$Dco7(.5, Tin) = 1.12396 \cdot \text{sec}^{-1} \cdot \text{cm}^2 \quad Pref = 1 \cdot \text{atm}$$

$$Dc7h14(.5, Tin) = 0.11846 \cdot \text{sec}^{-1} \cdot \text{cm}^2 \quad P = 3 \cdot \text{atm}$$



Tdsp_idsp
750-K
800-K
850-K
900-K
950-K
1000-K
1050-K
1100-K
1150-K
1200-K

Dco1(.5, Tdsp_idsp)
9.90331 · 10 ⁻⁵ · m ² · sec ⁻¹
1.10324 · 10 ⁻⁴ · m ² · sec ⁻¹
1.2208 · 10 ⁻⁴ · m ² · sec ⁻¹
1.34291 · 10 ⁻⁴ · m ² · sec ⁻¹
1.46949 · 10 ⁻⁴ · m ² · sec ⁻¹
1.60044 · 10 ⁻⁴ · m ² · sec ⁻¹
1.73572 · 10 ⁻⁴ · m ² · sec ⁻¹
1.87523 · 10 ⁻⁴ · m ² · sec ⁻¹
2.01893 · 10 ⁻⁴ · m ² · sec ⁻¹
2.16675 · 10 ⁻⁴ · m ² · sec ⁻¹

$$DcoT(T) := \exp \left[\left(-10.80086 + 1.6357427 \cdot \ln \left(\frac{T}{K} \right) \right) - 28.157906 \cdot \frac{K}{T} \right] \cdot 10^{-4} \cdot \text{m}^2 \cdot \text{sec}^{-1}$$

$$Dco1(.5, Tav) = 1.47689 \cdot \text{sec}^{-1} \cdot \text{cm}^2$$

$$DcoT(Tav) = 1.47689 \cdot \text{sec}^{-1} \cdot \text{cm}^2$$

$$dreco := 17 \cdot \text{in}$$

$$dreco = 43.18 \cdot \text{cm}$$

$$Lrec := 3.5 \cdot \text{in}$$

$$dreci := 6 \cdot \text{in}$$

$$dreci = 15.24 \cdot \text{cm}$$

$$Lrec = 8.89 \cdot \text{cm}$$

$$M0 = 0.29601 \cdot \text{kg} \cdot \text{sec}^{-1}$$

$$Arecup := \pi \cdot \frac{dreco^2 - dreci^2}{4}$$

$$Arecup = 0.1282 \cdot \text{m}^2$$

$$Grec0 := \frac{M0}{Arecup}$$

$$Grec0 = 2.30904 \cdot \text{kg} \cdot \text{m}^{-2} \cdot \text{sec}^{-1}$$

$$G0 = 8.98749 \cdot \text{kg} \cdot \text{m}^{-2} \cdot \text{sec}^{-1}$$

$$Prec := 1 \cdot \text{atm}$$

$$pmixrec(T) := \frac{MWmix(0.5) \cdot Prec}{R \cdot T}$$

$$pmixrec(Tav) = 0.36422 \cdot \text{kg} \cdot \text{m}^{-3}$$

DIAPHRAGM NO.0

$$U_{rec}(T) := \frac{G_{rec0}}{\rho_{mixrec}(T)}$$

$$U_{rec}(T_{avg}) = 6.33964 \cdot m \cdot sec^{-1}$$

$$S_{coT}(T) := \frac{\mu_{mixT}(T)}{D_{coT}(T) \cdot \rho_{mixrec}(T)}$$

Schmidt numbers are independent of pressure

$$R_{rec4}(T) := \frac{G_{rec0} \cdot d_{cell4}}{\mu_{mixT}(T)}$$

$$R_{rec4}(T_{avg}) = 69.96214$$

$$R_{rec6}(T) := \frac{G_{rec0} \cdot d_{cell6}}{\mu_{mixT}(T)}$$

$$R_{rec6}(T_{avg}) = 56.37495$$

$$T_{avg} = 952.8725 \cdot K$$

$$c_{fricrec4}(T, z) := \frac{14.227}{R_{rec4}(T)} \left[1 + 0.046263 \cdot \left(R_{rec4}(T) \cdot \frac{d_{cell4}}{z} \right) \right]^{0.45363}$$

$$c_{fricrec6}(T, z) := \frac{14.227}{R_{rec6}(T)} \left[1 + 0.046263 \cdot \left(R_{rec6}(T) \cdot \frac{d_{cell6}}{z} \right) \right]^{0.45363}$$

Calculate monolith pressure drop in several monoliths with entrance effect:

$$\Delta P_{rec4}(T) := 4 \cdot c_{fricrec4}(T, L_{rec}) \cdot \frac{\rho_{mixrec}(T) \cdot \left(\frac{U_{rec}(T)}{d_{cell4}} \right)^2}{2} \cdot \frac{L_{rec}}{d_{cell4}}$$

$$\frac{\Delta P_{rec4}(T_{avg})}{P_{rec}} = 0.00557$$

$$\Delta P_{rec6}(T) := 4 \cdot c_{fricrec6}(T, L_{rec}) \cdot \frac{\rho_{mixrec}(T) \cdot \left(\frac{U_{rec}(T)}{d_{cell6}} \right)^2}{2} \cdot \frac{L_{rec}}{d_{cell6}}$$

$$\frac{\Delta P_{rec6}(T_{avg})}{P_{rec}} = 0.00898$$

$$Num_{avgrec6}(z) := 2.976 \cdot \left[1 + \left(\frac{7.6 \cdot z}{R_{rec6}(T_{avg}) \cdot S_{cT}(T_{avg}) \cdot d_{cell6}} \right)^{\frac{8}{3}} \right]^{\frac{1}{8}}$$

$$Num_{avgrec6}(L_{rec}) = 2.97616$$

$$Num_{avgrec4}(z) := 2.976 \cdot \left[1 + \left(\frac{7.6 \cdot z}{R_{rec4}(T_{avg}) \cdot S_{cT}(T_{avg}) \cdot d_{cell4}} \right)^{\frac{8}{3}} \right]^{\frac{1}{8}}$$

$$Num_{avgrec4}(L_{rec}) = 2.97649$$

$$Num_{avgrec7R6}(z) := 2.976 \cdot \left[1 + \left(\frac{7.6 \cdot z}{R_{rec6}(T_{avg}) \cdot S_{c7T}(T_{avg}) \cdot d_{cell6}} \right)^{\frac{8}{3}} \right]^{\frac{1}{8}}$$

$$Num_{avgrec7R6}(L_{rec}) = 2.98024$$

102280-0995560

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$$\text{Numavgrec7R4}(z) := 2.976 \cdot \left[1 + \left(\frac{7.6 \cdot z}{\text{Rrec4}(\text{Tavg}) \cdot \text{Sc7T}(\text{Tavg}) \cdot \text{dcell4}} \right)^{\frac{1}{3}} \right]^8$$

$$\text{Numavgrec7R6}(\text{Lrec}) = 2.98024$$

$$\text{NumavgreccoR6}(z) := 2.976 \cdot \left[1 + \left(\frac{7.6 \cdot z}{\text{Rrec6}(\text{Tavg}) \cdot \text{ScCoT}(\text{Tavg}) \cdot \text{dcell6}} \right)^{\frac{1}{3}} \right]^8$$

$$\text{NumavgR6}(\text{Lrec}) = 2.98441$$

$$\text{NumavgreccoR4}(z) := 2.976 \cdot \left[1 + \left(\frac{7.6 \cdot z}{\text{Rrec4}(\text{Tavg}) \cdot \text{ScCoT}(\text{Tavg}) \cdot \text{dcell4}} \right)^{\frac{1}{3}} \right]^8$$

$$\text{NumavgreccoR4}(\text{Lrec}) = 2.97663$$

The average (integral) Nusselt numbers at 1-atm with the larger flow cross section show very little contribution of the thermal entry length, i.e. the flow velocities and heat and mass transfer coefficients have values close to those in long channels.

Now determine CH₄, C₇H₁₄, and CO conversions in 400 and 600 cpi honeycombs, assuming 80% C₇H₁₄ conversion downstream of the combustion monolith and upstream of the turbine

$$\text{ych4rec6}(T, z) := \text{ych4}(\text{Tavg}, \text{Lhc}) \cdot \exp\left(\frac{-4 \cdot z \cdot \text{Numavgrec6}(z)}{\text{Rrec6}(T) \cdot \text{ScT}(T) \cdot \text{dcell6}}\right)$$

$$\frac{\text{ych4rec6}(\text{Tavg}, \text{Lrec})}{\text{ych4}(\text{Tavg}, \text{Lhc})} = 2.733018 \cdot 10^{-13}$$

$$\text{ych4rec6}(\text{Tin}, \text{Lrec}) = 0 \quad \text{ych4}(\text{Tavg}, \text{Lhc}) = 1.81356 \cdot 10^{-3} \quad \text{Bypass} = 0 \quad \text{Lhc} = 3.5 \cdot \text{in} \quad \text{Diao} = 9 \cdot \text{in}$$

$$\text{yc7h14rec6}(T, z) := 0.2 \cdot \text{yc7h14}(\text{Tavg}, \text{Lhc}) \cdot \exp\left(\frac{-4 \cdot z \cdot \text{Numavgrec7R6}(z)}{\text{Rrec6}(T) \cdot \text{Sc7T}(T) \cdot \text{dcell6}}\right)$$

$$\frac{\text{yc7h14rec6}(\text{Tin}, \text{Lrec})}{0.2 \cdot \text{yc7h14}(\text{Tavg}, \text{Lhc})} = 0.00057$$

$$\text{yc7h14rec6}(\text{Tin}, \text{Lrec}) = 3.42819 \cdot 10^{-8} \quad 0.2 \cdot \text{yc7h14}(\text{Tavg}, \text{Lhc}) = 5.99172 \cdot 10^{-5}$$

$$\text{ych4rec4}(T, z) := \text{ych4}(\text{Tavg}, \text{Lhc}) \cdot \exp\left(\frac{-4 \cdot z \cdot \text{Numavgrec4}(z)}{\text{Rrec4}(T) \cdot \text{ScT}(T) \cdot \text{dcell4}}\right)$$

$$\frac{\text{ych4rec4}(\text{Tavg}, \text{Lrec})}{\text{ych4}(\text{Tavg}, \text{Lhc})} = 6.945016 \cdot 10^{-9}$$

$$\text{ych4rec4}(\text{Tin}, \text{Lrec}) = 8.84152 \cdot 10^{-13}$$

$$\text{yc7h14rec4}(T, z) := 0.2 \cdot \text{yc7h14}(\text{Tavg}, \text{Lhc}) \cdot \exp\left(\frac{-4 \cdot z \cdot \text{Numavgrec7R4}(z)}{\text{Rrec4}(T) \cdot \text{Sc7T}(T) \cdot \text{dcell4}}\right)$$

$$\frac{\text{yc7h14rec4}(\text{Tin}, \text{Lrec})}{0.2 \cdot \text{yc7h14}(\text{Tavg}, \text{Lhc})} = 0.00773$$

$$\text{yc7h14rec4}(\text{Tin}, \text{Lrec}) = 4.63263 \cdot 10^{-7} \quad 0.2 \cdot \text{yc7h14}(\text{Tavg}, \text{Lhc}) = 5.99172 \cdot 10^{-5} \quad 0.4 \cdot 7 \cdot \text{yc7h14}(\text{Tavg}, \text{Lhc}) = 8.3884 \cdot 10^{-4}$$

102290-099550

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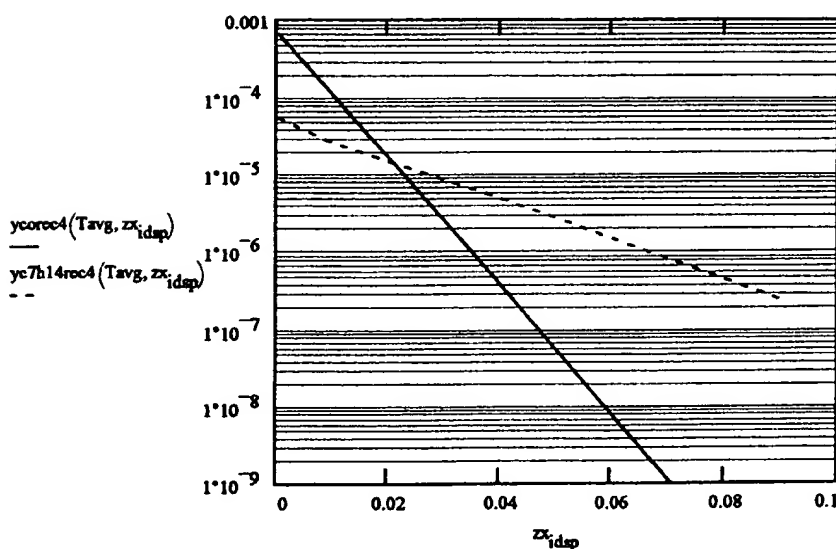
$$y_{corec4}(T, z) := 0.4 \cdot 7 \cdot y_{c7h14}(T_{avg}, L_{hc}) \cdot \exp\left(\frac{-4 \cdot z \cdot NumavgreccoK4(z)}{R_{rec4}(T) \cdot S_{ccoT}(T) \cdot d_{cell4}}\right)$$

$$y_{corec4}(T_{avg}, L_{rec}) = 3.06761 \cdot 10^{-11}$$

$$y_{corec6}(T, z) := 0.4 \cdot 7 \cdot y_{c7h14}(T_{avg}, L_{hc}) \cdot \exp\left(\frac{-4 \cdot z \cdot NumavgreccoR6(z)}{R_{rec6}(T) \cdot S_{ccoT}(T) \cdot d_{cell6}}\right)$$

$$y_{corec6}(T_{avg}, L_{rec}) = 2.9626 \cdot 10^{-15}$$

$$z_{x_{idsp}} := (idsp + 0.05) \cdot cm$$



$$Sc7T(T_{avg}) = 2.31842$$

$$S_{ccoT}(T_{avg}) = 0.73627$$

$$ScT(T_{avg}) = 0.67113$$

$$\frac{y_{corec4}(T_{avg}, L_{rec})}{(0.4 \cdot 7 \cdot y_{c7h14}(T_{avg}, L_{hc}))} = 3.65696 \cdot 10^{-8}$$

$$\frac{y_{corec6}(T_{avg}, L_{rec})}{(0.4 \cdot 7 \cdot y_{c7h14}(T_{avg}, L_{hc}))} = 3.53178 \cdot 10^{-12}$$

This analysis assumes 80% homogeneous conversion of fuel exiting a 3.5in. 600 cpi monolith without bypass flow and assuming 40% production of CO in the post combustion monolith region.

CO conversion in a 400 cpi recuperator monolith is >99.99%, while cyclohexane conversion is 99.2%.

The final CO and C7H14 levels are < 1 ppb and .5 ppm while post turbine concentrations are taken as 840 and 60 ppm respectively. CH4 conversion also should be very high and use of a 600 cpi or longer monolith would give higher HC conversions (x20 for 600 cpi).

Post turbine pre recuperation monolith pressure drops are modest: 0.56% for 400 cpi and 0.90% for 600 cpi monoliths.

102280" E99EE660

An alternative method of calculating performance uses local Nusselt numbers for heat and mass transfer to determine the wall temperature and combustion rates at the wall. First we define the local Nu function then check conversion assuming fast kinetics and compare with the previous averaged (integrated) Nu formula.

Local Nu(x) taken from Kays & Crawford for hydro & thermal entrance laminar with circular channel:

$$\text{Numono}(z) := (1 + \exp(-1.09689 - 0.381402 \cdot \ln(z) - 8.287774 \cdot z^{0.5})) \cdot 3.6 \text{Numono}(0.1152163) = 3.82723$$

$$\text{zzchar6} := \frac{\text{Rehc6}(\text{Tavg}) \cdot \text{Pr}(.5, \text{Tavg}) \cdot \text{dccll6}}{2}$$

$$\text{zzchar6} = 8.90257 \cdot \text{cm}$$

$$\frac{\text{Lhc}}{\text{zzchar6}} = 0.99859$$

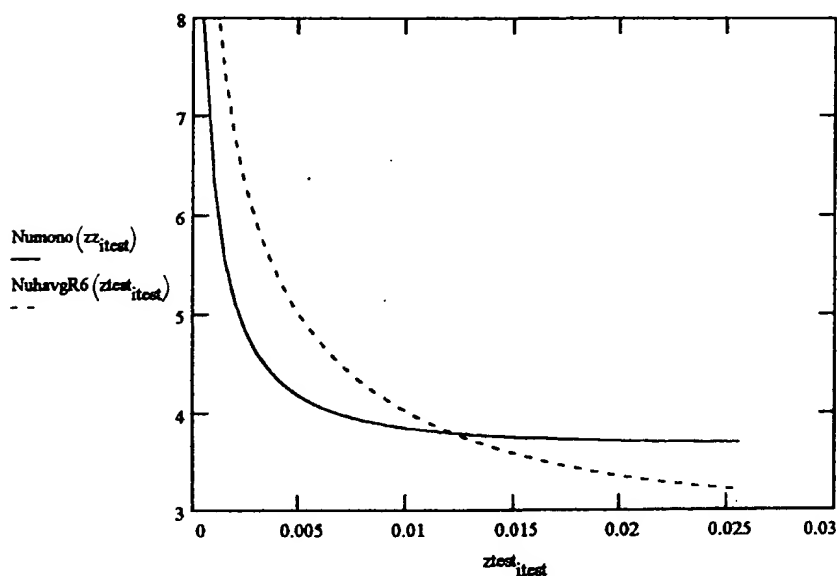
$$\text{Rehc6}(\text{Tavg}) = 252.34858$$

$$\text{itest} := 0..50$$

$$\text{dccll6} = 0.0967 \cdot \text{cm}$$

$$\text{ztest}_{\text{itest}} := \text{itest} \cdot 0.05 \cdot \text{cm} + 0.05 \cdot \text{cm}$$

$$\text{zz}_{\text{itest}} := \frac{\text{ztest}_{\text{itest}} + \text{dwall6}}{\text{zzchar6}}$$



$$\text{Rehc6}(\text{Tavg}) = 252.34858$$

$$\text{dccll6} = 0.0967 \cdot \text{cm}$$

$$\text{zz6ch4} := \frac{\text{Rehc6}(\text{Tavg}) \cdot \text{ScT}(\text{Tavg}) \cdot \text{dccll6}}{2}$$

$$\text{Pr}(.5, \text{Tavg}) = 0.72969$$

$$\text{Rehc6}(\text{Tavg}) \cdot \text{Pr}(.5, \text{Tavg}) \cdot \text{dccll6} = 17.80513 \cdot \text{cm}$$

$$\text{zz6c7h14} := \frac{\text{Rehc6}(\text{Tavg}) \cdot \text{Sc7T}(\text{Tavg}) \cdot \text{dccll6}}{2}$$

$$h(T, z) := \frac{\lambda_{\text{mixT}}(T) \cdot \text{Numono}\left(\frac{z}{\text{zzchar6}}\right)}{\text{dccll6}}$$

$$\text{kgpb}(T, z) := \frac{\text{Dch4T}(T) \cdot \text{Numono}\left(\frac{z}{\text{zz6ch4}}\right)}{\text{dccll6}}$$

$$\text{kgpb}(\text{Tim}, \text{Lhc}) = 15.5934 \cdot \text{sec}^{-1} \cdot \text{cm}$$

$$kgpb7(T, z) := \frac{Dc7h14T(T) \cdot Numono\left(\frac{z}{zz6c7h14}\right)}{dcell6}$$

$$kgpb7(Tin, Lhc) = 4.50626 \cdot \text{sec}^{-1} \cdot \text{cm}$$

Prater Temperature for CH4 at the inlet with fully developed flow

$$kgpb7(Tin, Lhc) \cdot \frac{P}{R \cdot Tin} \cdot \frac{ych40 - \Delta H_{comb}(Tin)}{h(Tin, Lhc)} = 309.73474 \cdot K$$

Prater Temperature for C7H14 at the inlet with fully developed flow

$$kgpb7(Tin, Lhc) \cdot \frac{P}{R \cdot Tin} \cdot \frac{y0c7h14 - \Delta H_{comb7}(Tin)}{h(Tin, 10\text{-cm})} = 90.38489 \cdot K$$

Determine maximum conversion of fuels with very fast catalytic combustion rates (zero fuel concentration at the wall)

$$iz := 0..100 \quad ych46_0 := ych40 \quad yc7h146_0 := y0c7h14 \quad T_{avg} := \frac{Tin + Tout}{2}$$

$$z6_{iz} := d_{wall6} + iz \cdot \frac{Lhc}{100} \cdot \frac{7}{7}$$

$$Lhc \cdot \frac{7}{7} = 8.89 \cdot \text{cm}$$

3.5 & 4-in. monolith length

$$ych46_{iz+1} := \left(1 - kgpb7(T_{avg}, z6_{iz}) \cdot \frac{Lhc}{100} \cdot \frac{7}{7} \cdot \frac{4}{dcell6} \cdot \frac{ecell6}{U(T_{avg})}\right) \cdot ych46_{iz}$$

$$\frac{ych46_{101}}{ych40} = 1.2447 \cdot 10^{-4}$$

$$\frac{ych4(T_{avg}, Lhc \cdot \frac{7}{7})}{ych40} = 0.00153$$

$$yc7h146_{iz+1} := \left(1 - kgpb7(T_{avg}, z6_{iz}) \cdot \frac{Lhc}{100} \cdot \frac{7}{7} \cdot \frac{4}{dcell6} \cdot \frac{ecell6}{U(T_{avg})}\right) \cdot yc7h146_{iz}$$

$$\frac{yc7h146_{101}}{y0c7h14} = 0.06145$$

By-pass length yC7H14out/yin yCH4out/yin

0 3.5-in 0.06145 $1.2447 \cdot 10^{-4}$

0 4-in 0.04256 $3.288 \cdot 10^{-5}$

0.2 3.5-in 0.0502 $5.96324 \cdot 10^{-5}$

0.2 4-in 0.03374 $1.3974 \cdot 10^{-5}$

0.4 3.5-in 0.02054 $2.17587 \cdot 10^{-6}$

0.4 3.5-in 0.01207 $2.92928 \cdot 10^{-7}$

$$T_{avg} = 952.8725 \cdot K$$

$$Lhc = 3.5 \cdot \text{in}$$

$$Dia0 = 9 \cdot \text{in}$$

$$\text{Bypass} = 0$$

Nu function with circular channel hydrothermal entry length shows 93.9% to 98.8% conversion of C7H14

102230-5962201

Packed bed

DAPE FONG MCD

Pressure Drop Calculations for a Packed Bed

given: ϵ - void fraction;
 d_p - effective particle diameter
 U - mean superficial velocity
 ν - kinematic viscosity
 ρ - density

$$f_{bed}(x) := \frac{150}{x} + 1.75$$

$$x = \frac{U \cdot d_p}{\nu}$$

1161 F

At $T = 900K$ and 10 atm pressure,

$$\rho_{mix}(0.0, 300-K) = 3.47058 \cdot kg \cdot m^{-3}$$

$$\rho_{mix}(.5, T_{avg}) = 1.09267 \cdot kg \cdot m^{-3}$$

$$\nu_{mix}(.5, T_{avg}) = 0.00004 \cdot m^2 \cdot sec^{-1}$$

$$j := 0..3$$

$$dp_j := \frac{.125}{j+1} \cdot in$$

$$\epsilon := 0.5$$

$$L_{bed} = 0.75 \cdot m$$

$$u0 := \nu_{mix}(.5, T_{avg})$$

$$dp = \begin{bmatrix} 0.3175 \\ 0.15875 \\ 0.10583 \\ 0.07938 \end{bmatrix} \cdot cm$$

$$i := 1..10$$

$$U_{tx_i} := i \cdot m \cdot sec^{-1}$$

$$\rho0 := \rho_{mix}(.5, T_{avg})$$

$$Re_{bed_{i,j}} := U_{tx_i} \cdot \frac{dp_j}{u0 \cdot (1 - \epsilon)}$$

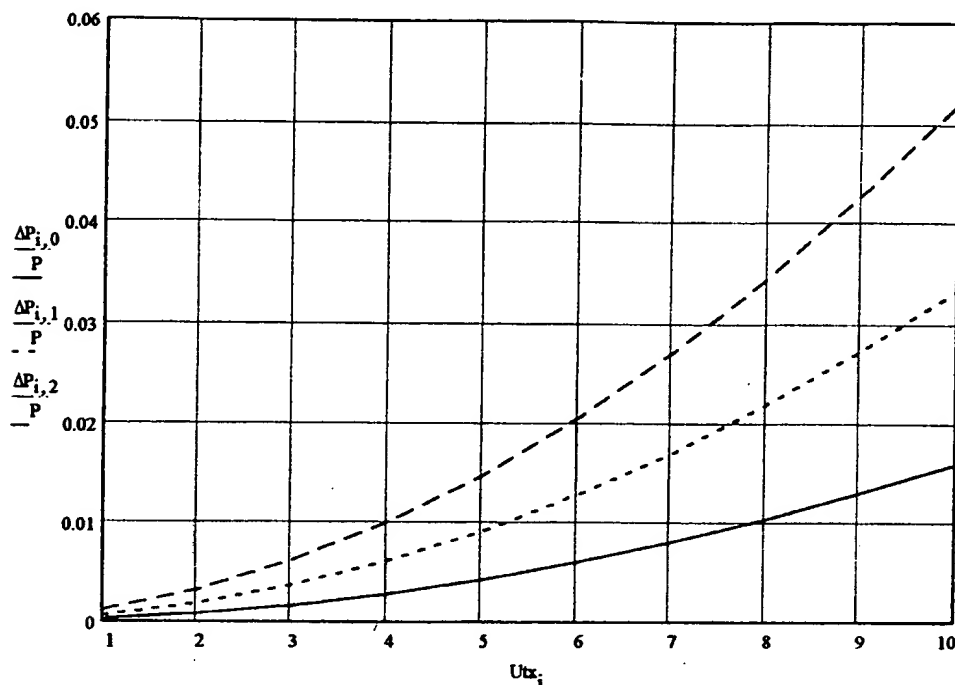
$$\Delta P_{i,j} := L_{bed} \cdot f_{bed}(Re_{bed_{i,j}}) \cdot \frac{1 - \epsilon}{\epsilon^3} \cdot \frac{\rho0 \cdot (U_{tx_i})^2}{dp_j}$$

102280" E96EE660

Utx =	0	0	0	0
1	175.19103	87.59551	58.39701	43.79776
2	350.38206	175.19103	116.79402	87.59551
3	525.57309	262.78654	175.19103	131.39327
4	700.76412	350.38206	233.58804	175.19103
5	875.95515	437.97757	291.98505	218.98875
6	1051.14617	525.57309	350.38206	262.78654
7	1226.3372	613.1686	408.77907	306.5843
8	1401.52823	700.76412	467.17608	350.38206
9	1576.71926	788.35963	525.57309	394.17982
10	1751.91029	875.95515	583.9701	437.97757

Rebed =	0	0	0	0
1	0.00067	0.00179	0.00335	0.00536
2	0.00226	0.0054	0.00943	0.01434
3	0.00474	0.01081	0.01822	0.02695
4	0.00814	0.01804	0.02972	0.04318
5	0.01243	0.02708	0.04395	0.06304
6	0.01764	0.03794	0.0609	0.08651
7	0.02375	0.0506	0.08056	0.11362
8	0.03077	0.06508	0.10294	0.14435
9	0.03869	0.08137	0.12804	0.1787
10	0.04752	0.09947	0.15586	0.21668

atm



Particle diameter
 $dp_2 = 0.04167 \text{ in } \frac{1}{24}''$

5 in 1 mm

$dp_1 = 0.0625 \text{ in } \frac{1}{16}''$

$dp_0 = 0.125 \text{ in}$

$L_{bed} = 0.75 \text{ in}$

$$\Delta P(\epsilon, T, z) := z \cdot f_{bed} \left[\frac{U_{bed}(T) \cdot dp_j}{\nu_0 \cdot (1 - \epsilon)} \right] \cdot \frac{1 - \epsilon}{\epsilon^3} \cdot \frac{\rho_0 \cdot (U_{bed}(T))^2}{dp_j}$$

$$\epsilon := 0.45$$

$$dp = \begin{bmatrix} 0.3175 \\ 0.15875 \\ 0.10583 \\ 0.07938 \end{bmatrix} \text{ cm}$$

$$\Delta P(.45, T_{avg}, L_{bed})$$

P

0.00173
0.00407
0.00703
0.0106

$$\Delta P(.5, T_{avg}, L_{bed})$$

P

0.00113
0.00263
0.00449
0.00673

$$U_{bed}(T_{avg}) = 2.5 \text{ m} \cdot \text{sec}^{-1}$$

For larger particles use axial beds with greater length

$$k := 0$$

$$dp_0 = 0.125 \text{ in}$$

$\frac{1}{2}''$

$\frac{1}{8}''$

what we have

$$U(T_{avg}) = 8.22528 \text{ m} \cdot \text{sec}^{-1}$$

$$\Delta P_{axial}(\epsilon, T, z) := z \cdot f_{bed} \left[\frac{U(T) \cdot dp_k}{\nu_0 \cdot (1 - \epsilon)} \right] \cdot \frac{1 - \epsilon}{\epsilon^3} \cdot \frac{\rho_0 \cdot (U(T))^2}{dp_k}$$

$$\Delta P_{axial}(\epsilon, T_{avg}, 1 \text{ in}) = 0.0657 \text{ atm}$$

$$P = 3 \text{ atm}$$

$$\frac{\Delta P_{axial}(\epsilon, T_{avg}, 1 \text{ in})}{P} = 0.0219$$

1/8th inch pellets give about 2% pressure drop per inch

Determine Nu values for heat and mass transfer between particles and the gas phase in the bed

$$\text{Repart}(T) := \frac{U_{\text{bed}}(T) \cdot dp}{v_{\text{mix}}(T) \cdot (1 - \epsilon)}$$

$$dp = \begin{bmatrix} 0.3175 \\ 0.15875 \\ 0.10583 \\ 0.07938 \end{bmatrix} \cdot \text{cm} \quad \epsilon = 0.45$$

$$\text{Repart}(T_{\text{avg}}) = \begin{bmatrix} 398.16156 \\ 199.08078 \\ 132.72052 \\ 99.54039 \end{bmatrix}$$

$$\text{Pr}(.5, T_{\text{avg}}) = 0.72969$$

$$\text{Sc}(.5, T_{\text{avg}}) = 0.67112$$

$$k := 0$$

$$\text{NuhpartR}(T) := 1.34 \cdot \left[\text{Pr}(.5, T)^{0.4} \cdot \left[0.4 \cdot (\text{Repart}(T)_k)^{0.5} + 0.2 \cdot (\text{Repart}(T)_k)^2 \right] \right]$$

$$\text{NuhpartR}(T_{\text{avg}}) = 22.21552$$

$$\text{havgpart}(T) := \frac{\lambda_{\text{mix}}(T) \cdot \text{NuhpartR}(T)}{dp_k}$$

$$\text{havgpart}(T_{\text{avg}}) = 445.59219 \cdot \text{m}^{-2} \cdot \text{K}^{-1} \cdot \text{W}$$

Effective boundary
layer thickness:

$$\frac{dp_k}{\text{NuhpartR}(T_{\text{avg}})} = 142.9181 \cdot \mu\text{m}$$

$$\frac{d_{\text{cell6}}}{\text{NuhavgR6}(\text{Lhc})} = 323.77508 \cdot \mu\text{m}$$

$$dp_k = 0.3175 \cdot \text{cm}$$

$$d_{\text{cell6}} = 0.0967 \cdot \text{cm}$$

$$\text{NumpartR}(T) := 1.34 \cdot \text{Sc}(T)^{0.4} \cdot \left[0.4 \cdot (\text{Repart}(T)_k)^2 + 0.2 \cdot (\text{Repart}(T)_k)^3 \right]$$

$$\text{NumpartR}(T_{\text{avg}}) = 21.48438$$

$$\text{kgpart}(T) := \frac{D_{\text{ch4}}(T) \cdot \text{NumpartR}(T)}{\epsilon \cdot dp_k}$$

$$\text{kgpart}(T_{\text{in}}) = 72.76151 \cdot \text{sec}^{-1} \cdot \text{cm}$$

$$\text{Nupart7R}(T) := 1.34 \cdot \text{Sc7}(T)^{0.4} \cdot \left[0.4 \cdot (\text{Repart}(T)_k)^{0.5} + 0.2 \cdot (\text{Repart}(T)_k)^2 \right]$$

$$\text{Nupart7R}(T_{\text{avg}}) = 35.27582$$

$$\text{kgfb7}(T) := \frac{D_{\text{c7h14}}(T) \cdot \text{Nupart7R}(T)}{\epsilon \cdot dp_k}$$

$$\text{kgfb7}(T_{\text{in}}) = 34.44665 \cdot \text{sec}^{-1} \cdot \text{cm}$$

102230-595566

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$$ych46_{iz+1} := \left[1 - kgpart(Tavg) \cdot \frac{Lbed}{50} \cdot \frac{6 \cdot (1 - \epsilon)^2}{dp_k} \cdot \frac{1}{Ubed(Tavg)} \right] ych46_{iz}$$

$$\frac{ych46_{51}}{ych46_0} = 0.02369771$$

$$ych4p(T, z) := ych40 \cdot \exp \left[-6 \cdot (1 - \epsilon) \cdot \frac{NumpartR(T)}{\epsilon \cdot Repart(T)_k \cdot ScT(T)} \cdot \frac{z}{dp_k} \right]$$

$$\frac{ych4p(Tavg, Lbed)}{ych40} = 0.02908261$$

$$yc7h14(T, z) := y0c7h14 \cdot \exp \left[-6 \cdot (1 - \epsilon) \cdot \frac{Nupart7R(T)}{\epsilon \cdot Repart(T)_k \cdot Sc7T(T)} \cdot \frac{z}{dp_k} \right]$$

$$\frac{yc7h14(Tavg, Lbed)}{y0c7h14} = 0.18611$$

[REDACTED]

$$dp_k = 0.3175 \cdot \text{cm}$$

dpart(cm)	yout/yinC7H14	yout/yinCH4	ΔP/P
0.3175	0.18611	0.02908261	0.00113
0.15875	0.0116	0.0000846	0.00263

$$Ubed(Tavg) = 2.5 \cdot \text{m} \cdot \text{sec}^{-1}$$

$$\epsilon = 0.45$$

$$Wbed = 17.78 \cdot \text{cm}$$

$$Lbed = 1.905 \cdot \text{cm}$$

Determine hydrocarbon conversions in the packed beds vs pressure to estimate effective conversion at equivalent pressure drop

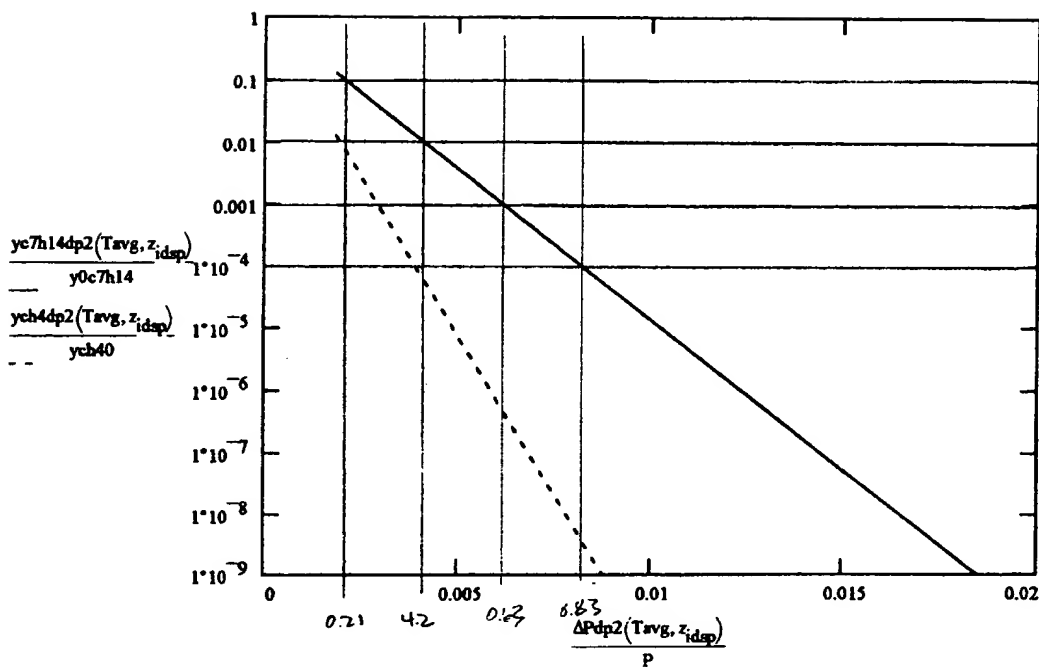
$$yc7h14dp2(T, z) := y0c7h14 \cdot \exp \left[-6 \cdot (1 - \epsilon) \cdot \frac{1.34 \cdot Sc7T(T)^{0.4} \cdot \left[0.4 \cdot (Repart(T)_2)^2 + 0.2 \cdot (Repart(T)_2)^3 \right]}{\epsilon \cdot Repart(T)_2 \cdot Sc7T(T)} \cdot \frac{z}{dp_2} \right]$$

$$ych4dp2(T, z) := ych40 \cdot \exp \left[-6 \cdot (1 - \epsilon) \cdot \frac{1.34 \cdot ScT(T)^{0.4} \cdot \left[0.4 \cdot (Repart(T)_2)^2 + 0.2 \cdot (Repart(T)_2)^3 \right]}{\epsilon \cdot Repart(T)_2 \cdot ScT(T)} \cdot \frac{z}{dp_2} \right]$$

$$\Delta Pdp2(Tavg, z) := z \cdot fbed(Repart(Tavg)_2) \cdot \frac{1 - \epsilon \cdot \rho 0 \cdot (Ubed(Tavg))^2}{\epsilon^3 \cdot dp_2}$$

$$Ubed(Tavg) = 2.5 \cdot \text{m} \cdot \text{sec}^{-1}$$

102280" E99E660



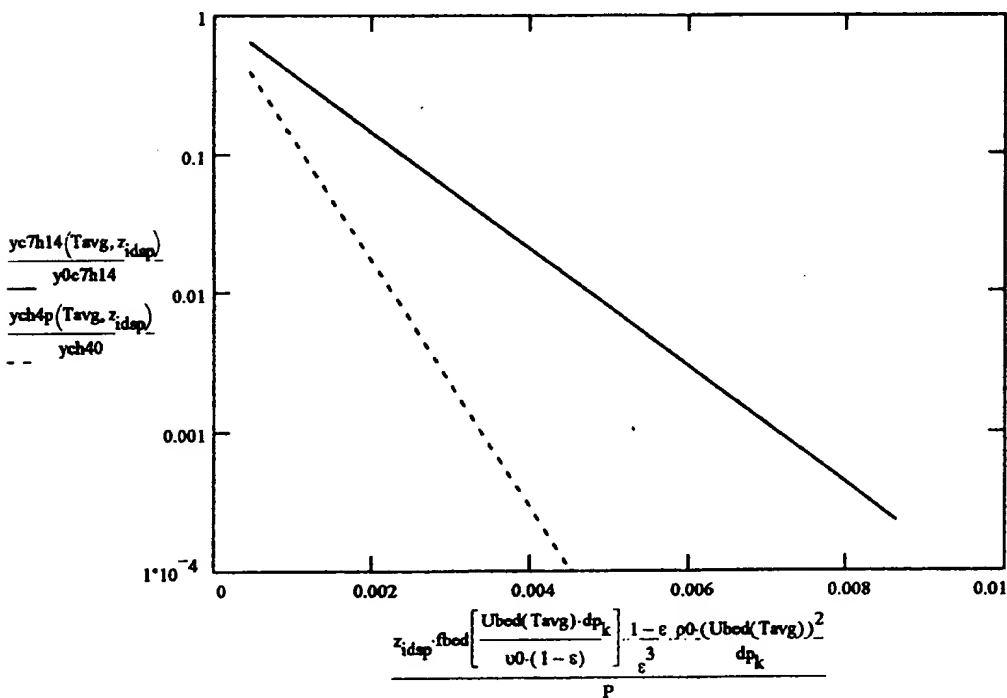
Small

$$dp_2 = 0.10583 \text{ cm}$$

$$dp_2 = 0.04167 \text{ in}$$

$$z_9 = 3.74016 \text{ in}$$

$$L_{bed} = 0.75 \text{ in}$$



Large

$$dp_0 = 0.3175 \text{ cm}$$

$$dp_0 = 0.125 \text{ in}$$

$$z_9 = 3.74016 \text{ in}$$

$$L_{bed} = 0.75 \text{ in}$$

$$U_{bed}(T_{avg}) = 2.5 \text{ m} \cdot \text{sec}^{-1}$$

For oblique flow through cone-shaped beds, large particles give a very low ΔP (even with thick beds) and high conversion

CAPTION: NCC

$$z_{cx} := 2.71 \cdot \text{cm}$$

$$\frac{\Delta P_{dp2}(T_{avg}, z_{cx})}{P} = 0.01000$$

$$\frac{y_{c7h14dp2}(T_{avg}, z_{cx})}{y_{0c7h14}} = 1.32434 \cdot 10^{-3}$$

$$\frac{y_{ch4dp2}(T_{avg}, z_{cx})}{y_{ch40}} = 5.45793 \cdot 10^{-11}$$

For $\Delta P/P = 1\%$, C7H14 conversion = 99.9987% with fine particles, $dp = 1.06 \text{ mm}$

$$z_y := 2.0 \cdot \text{cm}$$

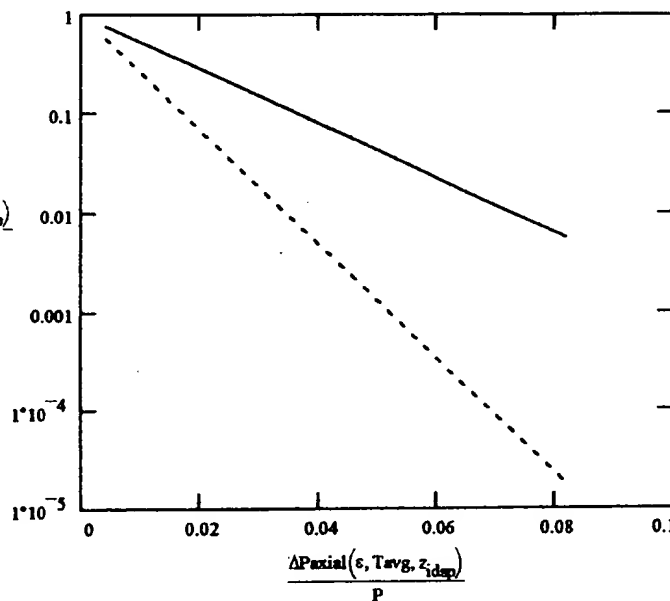
$$\text{Repaxial}(T) := \frac{U(T) \cdot dp_0}{v_{mixT}(T) \cdot (1 - \epsilon)}$$

$$\text{Numpaxial}(T) := 1.34 \cdot \text{ScT}(T)^{0.4} \cdot \left[0.4 \cdot (\text{Repaxial}(T))^2 + 0.2 \cdot (\text{Repaxial}(T))^3 \right]$$

$$\text{Nump7axial}(T) := 1.34 \cdot \text{Sc7T}(T)^{0.4} \cdot \left[0.4 \cdot (\text{Repaxial}(T))^2 + 0.2 \cdot (\text{Repaxial}(T))^3 \right]$$

$$y_{ch4paxial}(T, z) := y_{ch40} \cdot \exp \left[-6 \cdot (1 - \epsilon) \cdot \frac{\text{Numpaxial}(T)}{\epsilon \cdot \text{Repaxial}(T) \cdot \text{ScT}(T)} \cdot \frac{z}{dp_0} \right]$$

$$y_{c7h14paxial}(T, z) := y_{0c7h14} \cdot \exp \left[-6 \cdot (1 - \epsilon) \cdot \frac{\text{Nump7axial}(T)}{\epsilon \cdot \text{Repaxial}(T) \cdot \text{Sc7T}(T)} \cdot \frac{z}{dp_0} \right]$$



Pressure drop increases approximately with the square of flow velocity while conversion decreases exponentially

$$U(T_{avg}) = 8.22528 \cdot \text{m} \cdot \text{sec}^{-1}$$

$$z_y := 2.32 \cdot \text{cm}$$

$$\frac{\Delta P_{axial}(\epsilon, T_{avg}, z_y)}{P} = 0.02000$$

$$\frac{y_{ch4paxial}(T_{avg}, z_y)}{y_{ch40}} = 0.06888284$$

$$\frac{y_{c7h14paxial}(T_{avg}, z_y)}{y_{0c7h14}} = 0.28038$$

For flow perpendicular to the fixed bed, even with large catalyst particles, the equivalent pressure drop for high C7H14 conversion is very high. Even with $\Delta P/P = 2\%$, the C7H14 conversion is only 72%. For high conversion with practical fixed beds, the superficial bed flow rate must lower than about 3 m/sec to give high conversion with low ΔP

CAPSTONE MCD

Define Catalyst Functions:

$$R = 82.07601 \cdot K^{-1} \cdot atm \cdot cm^3 \quad atm \cdot cm^3 / mol \cdot K$$

$$TOL := 0.0001$$

$$R_{cm} := 83143000 \cdot gm \cdot cm^2 \cdot sec^{-2} \cdot K^{-1}$$

$$\eta_{sph}(\phi) := \frac{3}{\phi} \cdot \left(\frac{1}{\tanh(\phi)} - \frac{1}{\phi} \right)$$

$$\eta_{fpl}(\phi) := \frac{\tanh(\phi)}{\phi}$$

Physical Properties for Pd/Al₂O₃ Washcoated cCatalyst

$$Scat := 85 \cdot m^2 \cdot gm^{-1}$$

$$\rho_{catpart} := 2.5 \cdot gm \cdot cm^{-3}$$

$$V_{\mu pore} := 0.15 \cdot cm^3 \cdot gm^{-1}$$

$$Loat := 0.0020 \cdot cm$$

$$d_{pcat} := 0.0002 \cdot cm$$

Washcoat thickness - 20 microns

Size of γ -Al₂O₃ particle within washcoat - 2 microns

$$d_{\mu pore} := 6 \cdot \frac{V_{\mu pore}}{Scat}$$

$$\epsilon_{\mu pore} := 0.375$$

$$d_{\mu pore} = 1.05882 \cdot 10^{-6} \cdot cm$$

$$\tau_{\mu pore} := 3.0$$

$$DeffCH4(x, T) := \frac{\frac{\epsilon_{\mu pore}}{\tau_{\mu pore}}}{\frac{1}{Dch4(x, T)} + \frac{3}{d_{\mu pore} \cdot \sqrt{\frac{8 \cdot R \cdot T}{\pi \cdot MW_0}}}}$$

$$d_{\mu pore} \cdot \sqrt{\frac{8 \cdot R \cdot T_{in}}{\pi \cdot MW_0}} = 0.10953 \cdot sec^{-1} \cdot cm^2$$

$$Dch4(.5, T_{in}) = 0.41195 \cdot sec^{-1} \cdot cm^2$$

$$DeffCH4(.5, T_{in}) = 0.00419 \cdot sec^{-1} \cdot cm^2$$

$$DeffC7H14(x, T) := \frac{\frac{\epsilon_{\mu pore}}{\tau_{\mu pore}}}{\frac{1}{Dc7h14(x, T)} + \frac{3}{d_{\mu pore} \cdot \sqrt{\frac{8 \cdot R \cdot T}{\pi \cdot MW_6}}}}$$

$$d_{\mu pore} \cdot \sqrt{\frac{8 \cdot R \cdot T_{in}}{\pi \cdot MW_6}} = 0.04428 \cdot sec^{-1} \cdot cm^2$$

$$Dc7h14(.5, T_{in}) = 0.11846 \cdot sec^{-1} \cdot cm^2$$

$$DeffC7H14(0.5, T_{in}) = 0.00164 \cdot sec^{-1} \cdot cm^2$$

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[REDACTED]

$$D_{\text{macCH}_4}(.5, 800 \cdot K) = 0.06442 \cdot \text{sec}^{-1} \cdot \text{cm}^2$$

$$D_{\text{macC7H14}}(.5, 800 \cdot \text{K}) = 0.01851 \cdot \text{sec}^{-1} \cdot \text{cm}^2$$

Macropore porosity - 0.4 and tortuosity - 2.5

$$\phi\mu(k0T,.5,T_{im}) = 0.021$$
$$\Phi_{\text{mac}}(\text{k0T}, \text{ych40}, \text{Tin}) = 0.31774$$
$$\phi_7(k_0T, .5, T_{im}) = 0.03357$$
$$\Phi_{\text{mac7}}(\text{kOT}, \text{ych40}, \text{Tin}) = 0.59265$$

$$\text{Rate}_{\text{CH}_4}(\text{kOT}, 0, T_{\text{in}}) = -1610.07113 \cdot \text{sec}^{-1}$$

$$\text{Rate}_{\text{C7H14}}(\text{kOT}, 0, T_{\text{in}}) = -1492.98186 \cdot \text{sec}^{-1}$$

Defines transport restricted rate constant function given catalyst effective first order rate constant - k_0T , methane or cyclohexane conversion - x , and surface temperature - T

$$T_s := T_{in} \quad k_0T = 0.01 \cdot \text{sec}^{-1} \cdot \text{gm}^{-1} \quad T_{avg} = 952.8725 \cdot \text{K}$$

$$\text{kgpb}(T_{in}, 0.1 \cdot \text{cm}) = 26.77306 \cdot \text{sec}^{-1} \cdot \text{cm} \quad \text{RatekCH4}(k_0T, 0, T_s) = -1610.07113 \cdot \text{sec}^{-1} \quad \text{Lcat} = 0.002 \cdot \text{cm}$$

$$T_{in} + \frac{\text{kgpb}(T_{avg}, 0.1 \cdot \text{cm})}{\left[\left(\frac{\text{kgpb}(T_{avg}, 1 \cdot \text{cm})}{- \text{RatekCH4}(k_0T, 0, T_s) \cdot \text{Lcat}} \right) + 1 \right]} \cdot \frac{\text{ych40} \cdot \Delta H_{\text{comb}}(T_{avg})}{h(T_{avg}, 1 \cdot \text{cm})} \cdot \frac{P}{R \cdot T_s} = 840.46756 \cdot \text{K} \quad T_{out} = 1094.817 \cdot \text{K}$$

$$x_s := \text{ych40} \quad x_s = 0.01183 \quad T_{in} = 810.928 \cdot \text{K}$$

$$Rk := 6.33 \cdot \text{m}^{-2} \cdot \text{sec}^{-1} \quad \text{Ratech4} := 0.036 \cdot \text{m}^{-2} \cdot \text{sec}^{-1} \quad k_0T = 10 \cdot \text{kg}^{-1} \cdot \text{sec}^{-1}$$

Set up subroutine/function to solve for the surface temperature given a rate constant

$$\text{TOL} := 0.0001 \quad \text{ych40} = 0.01183 \quad x := 0.01$$

$$T_s := 1673 \cdot \text{K} \quad T_{s7} := 1473 \cdot \text{K}$$

Given

$$T_s = T_{in} + \frac{y(\text{ych40}, x)_0 \cdot \frac{P}{R \cdot T_s} - \Delta H_{\text{comb}}(T_s)}{\frac{1}{- \text{RatekCH4}(k_0T, x, T_s) \cdot \text{Lcat}} + \frac{1}{\text{kgpb}\left(T_{in}, \frac{\text{Lhc}}{100}\right)} h\left(T_{in}, \frac{\text{Lhc}}{100}\right)}$$

$$\text{Tshi}(k_0T) := \text{Find}(T_s) \quad \text{Tshi}(100 \cdot k_0T) = 1010.10631 \cdot \text{K}$$

Given

$$T_{s7} = T_{in} + \frac{y_7(y_0c_7h_{14}, x)_6 \cdot \frac{P}{R \cdot T_s} - \Delta H_{\text{comb}7}(T_s)}{\frac{1}{- \text{RatekC7H14}(k_0T, x, T_s) \cdot \text{Lcat}} + \frac{1}{\text{kgpb}7\left(T_{in}, \frac{\text{Lhc}}{100}\right)} h\left(T_{in}, \frac{\text{Lhc}}{100}\right)}$$

$$\text{Tshi7}(k_0T) := \text{Find}(T_{s7}) \quad \text{Tshi7}(100 \cdot k_0T) = 873.32275 \cdot \text{K}$$

$$Rk := - \text{RatekCH4}(k_0T, x_s, T_s) \cdot \text{Lcat}$$

$$Rk7 := - \text{RatekC7H14}(k_0T, x_s, T_s) \cdot \text{Lcat}$$

$$Rk = 6.72632 \cdot \text{sec}^{-1} \cdot \text{cm}$$

$$Rk7 = 6.41773 \cdot \text{sec}^{-1} \cdot \text{cm}$$

$$k_0T = 10 \cdot \text{kg}^{-1} \cdot \text{sec}^{-1}$$

$$\text{Ratech4} := \frac{x_s \cdot \frac{P}{R \cdot T_s}}{\frac{1}{Rk} + \frac{1}{\text{kgpb}(T_{in}, \text{Lhc})}}$$

$$\text{kgpb}(T_{in}, \text{Lhc}) = 15.5934 \cdot \text{sec}^{-1} \cdot \text{cm}$$

$$\text{Ratech4} = 0.01215 \cdot \text{m}^{-2} \cdot \text{sec}^{-1}$$

$$\text{kgpb7}(T_{in}, \text{Lhc}) = 4.50626 \cdot \text{sec}^{-1} \cdot \text{cm}$$

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$$T_s := T_{in} + \text{Ratech4} \cdot \frac{-\Delta H_{comb}(T_s)}{h(T_{in}, L_{hc})} \cdot y_{ch40}$$

$$\text{Ratech4} = 0.01215 \cdot \text{m}^{-2} \cdot \text{sec}^{-1}$$

$$x_s := \frac{\text{Ratech4}}{R_k}$$

$$R_k = 6.72632 \cdot \text{sec}^{-1} \cdot \text{cm}$$

$$T_s = 811.4626 \cdot \text{K}$$

$$x_s = 0.18057 \cdot \text{m}^{-3}$$

$$T_{in} = 810.928 \cdot \text{K}$$

$$k_0 T = 10 \cdot \text{kg}^{-1} \cdot \text{sec}^{-1}$$

$$T_{shi}(100 \cdot k_0 T) = 1010.10631 \cdot \text{K}$$

$$T_{shi}(0.01 \cdot \text{kg}^{-1} \cdot \text{sec}^{-1}) = 810.96346 \cdot \text{K}$$

$$T_{shi7}(100 \cdot k_0 T) = 873.32275 \cdot \text{K}$$

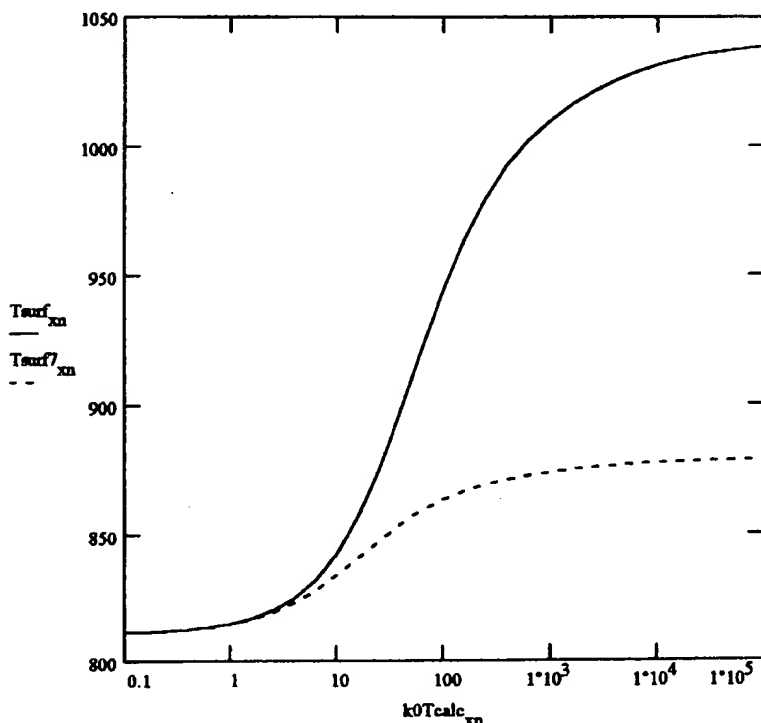
$$T_{shi7}(0.01 \cdot \text{kg}^{-1} \cdot \text{sec}^{-1}) = 810.96393 \cdot \text{K}$$

$$x_n := 0, 1..30$$

$$k_0 T_{calc_xn} := 10^{-1 + \frac{x_n}{5}} \cdot \text{kg}^{-1} \cdot \text{sec}^{-1}$$

$$T_{surf_xn} := T_{shi}(k_0 T_{calc_xn})$$

$$T_{surf7_xn} := T_{shi7}(k_0 T_{calc_xn})$$



This plot shows the surface temperature within a honeycomb channel as a function of the specific catalytic rate constant for methane and methylcyclohexane combustion at a location within 1-mm of the leading edge

Takes into account the internal pore diffusion (micro- and macropores) and boundary layer heat and mass transport. Upper surface temperature limit approaches the adiabatic temperature for methane and a much lower (Prater) temperature for C7H14

k0 unit - sec⁻¹ per kg washcoat
T unit - K

We can also determine the actual effective first order rate constants for methane, propane, and other fuels and estimate the temperatures required for catalytic light-off and extinction, with roughly estimated Nu numbers.

Other factors, such as the upstream surface temperature and gas phase radial temperature profile and thermal conduction of the catalyst wall, can also effect the light-off and the critical extinction points. These calculations are beyond the scope of the current analysis.

PdO Catalyst Rate Constants

$$\text{Erpd0} := 12800 \cdot \text{K}$$

$$\text{Erpd1} := 4900 \cdot \text{K}$$

$$\text{Erpd3} := 15000 \cdot \text{K}$$

Region0 - low T PdO to 625K
ignores inhibition by H₂O and CO₂

Region1 - Intermediate T
625K to 909K

Region2 - Flat 909K
to 1048K decomposition

Region3 -
Pd metal

$$\text{Apd0} := 2.4 \cdot 10^3 \cdot 200 \cdot \text{gm}^{-1} \cdot \text{sec}^{-1}$$

$$\text{Apd3} := \text{Apd2} \cdot \exp\left(\frac{\text{Erpd3}}{1048.1 \cdot \text{K}}\right)$$

$$\text{Apd1} := \text{Apd0} \cdot \exp\left(-\frac{\text{Erpd0}}{625 \cdot \text{K}} + \frac{\text{Erpd1}}{625 \cdot \text{K}}\right)$$

$$\text{Apd2} := \text{Apd1} \cdot \exp\left(\frac{-\text{Erpd1}}{909.1 \cdot \text{K}}\right)$$

Interpolation formula for the four PdO+Pd rate constants

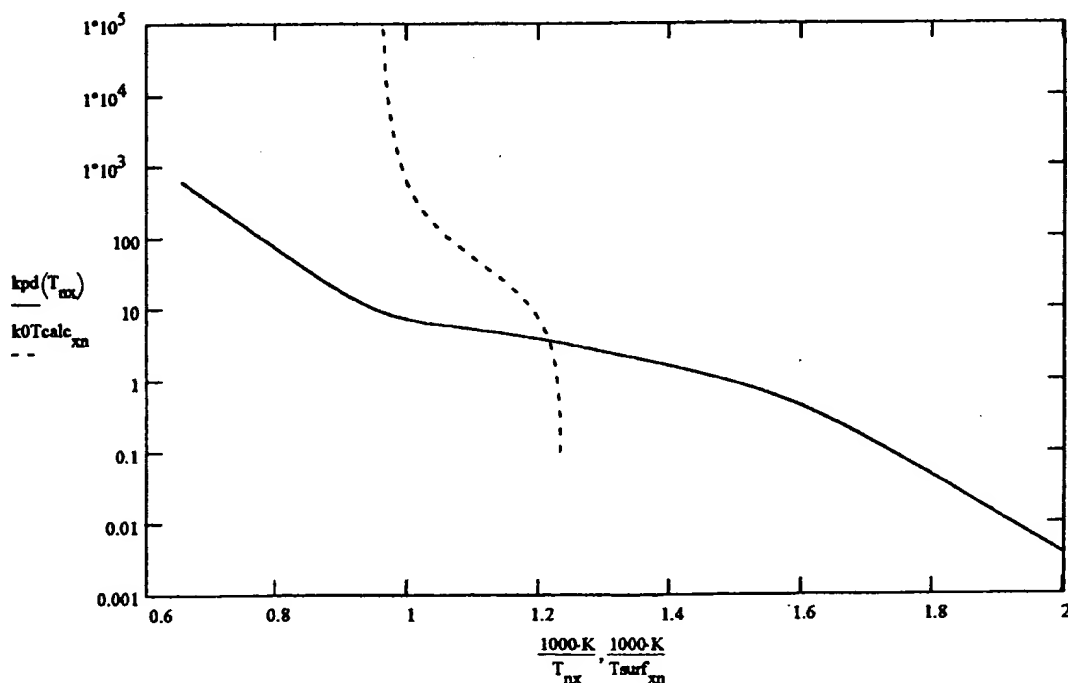
$$\text{kpd}(T) := \left[\text{Apd3}^2 \cdot \exp\left(-\frac{2 \cdot \text{Erpd3}}{T}\right) + \frac{1}{\left(\text{Apd2}^{-2} + \text{Apd1}^{-2} \cdot \exp\left(\frac{2 \cdot \text{Erpd1}}{T}\right) + \text{Apd0}^{-2} \cdot \exp\left(\frac{2 \cdot \text{Erpd0}}{T}\right) \right)} \right]^{0.5}$$

$$n_x := 0, 1, \dots, 41 \quad T_{n_x} := 500 \cdot \text{K} + n_x \cdot 25 \cdot \text{K}$$

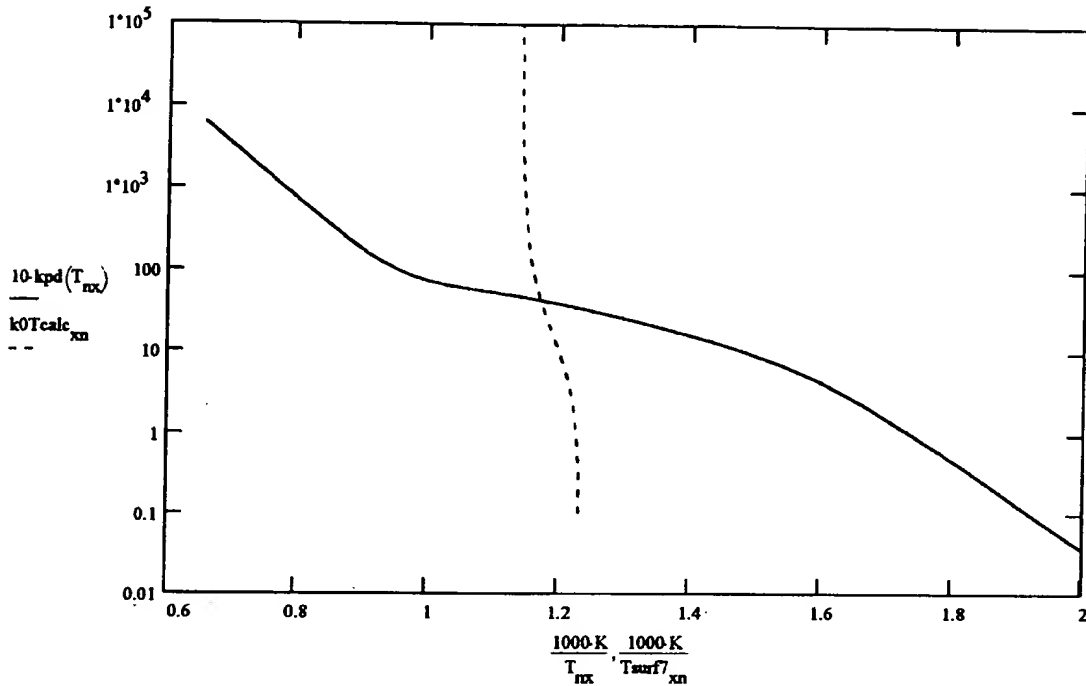
CATALYTIC RATE CONSTANT NEEDED FOR HEAT BALANCE IN A MONOLITH WITH FULLY DEVELOPED FLOW

Compared with extrapolated but measured rate constants (mol/atmCH₄/s/gcat)

$$L_{\text{cat}} = 0.00002 \cdot \text{m}$$



Compared with extrapolated and estimated
rate constants for C7H14 (10x mol/atmCH4/s/gcat)



Define functions to calculate surface temperature profiles given gas temperature and composition

$$TOL := 0.1 \quad Ts = 811.4626 \cdot K$$

$$x = 0.01$$

$$Tsx := 1500 \cdot K \quad Tsx7 := 1400 \cdot K$$

$$\frac{1}{-RatekCH4(kpd(Tsx), x, Tsx) \cdot Lcat} + \frac{1}{kgpb(Tin, Lhc)} = 7.01896 \cdot m^{-1} \cdot sec$$

Given

$$Tsx = Tin + \frac{y(ych40, x)_0 \cdot \frac{P}{R \cdot Tsx} \cdot \frac{-\Delta H_{comb}(Tsx)}{h(Tin, z)}}{\frac{1}{-RatekCH4(kpd(Tsx), x, Tsx) \cdot Lcat} + \frac{1}{kgpb(Tin, z)}}$$

$$Tsrf(Tin, x, z) := Find(Tsx)$$

$$Tsch4x := Tsrf(Tin, x, 0.1 \cdot cm)$$

$$Z_{inlet} = 0.1 \cdot cm$$

$$Tsch4x = 823.23891 \cdot K$$

$$Tin = 810.928 \cdot K$$

$$x = 0.01$$

$$Lcat = 0.002 \cdot cm$$

$$y(ych40, x)_0 = 0.01171$$

$$kpd(Tsch4x) = 3.51311 \cdot kg^{-1} \cdot sec^{-1}$$

$$kgpb(Tin, 0.1 \cdot cm) = 26.77306 \cdot sec^{-1} \cdot cm$$

$$-RatekCH4(kpd(Tsch4x), x, Tsch4x) \cdot Lcat = 1.17316 \cdot sec^{-1} \cdot cm$$

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Given

$$T_{sx7} = T_{in} + \frac{y_7(y_{0c7h14}, x) \cdot \frac{P}{R \cdot T_{sx7}}}{\frac{1}{-Rate_{C7H14}(10 \cdot kpd(T_{sx7}), x, T_{sx7}) \cdot L_{cat}} + \frac{1}{kg_{pb7}(T_{in}, z)}} - \frac{\Delta H_{comb7}(T_{sx7})}{h(T_{in}, z)}$$

$$T_{srf7}(T_{in}, x, z) := \text{Find}(T_{sx7})$$

$$T_{sc7h14x} := T_{srf7}(T_{in}, x, 0.1 \cdot \text{cm})$$

$$Z_{inlet} = 0.1 \text{ cm}$$

$$T_{sc7h14x} = 871.51735 \cdot K$$

$$T_{in} = 810.928 \cdot K$$

$$x = 0.01$$

$$L_{cat} = 0.002 \cdot \text{cm}$$

$$y(y_{ch40}, x)_0 = 0.01171$$

$$10 \cdot kpd(T_{sc7h14x}) = 44.23122 \cdot \text{kg}^{-1} \cdot \text{sec}^{-1}$$

$$-Rate_{C7H14}(10 \cdot kpd(T_{sch4x}), x, T_{sc7h14x}) \cdot L_{cat} = 9.21644 \cdot \text{sec}^{-1} \cdot \text{cm}$$

$$kg_{pb7}(T_{in}, 0.1 \cdot \text{cm}) = 12.3599 \cdot \text{sec}^{-1} \cdot \text{cm}$$

Assuming the rate constant for C7H14 combustion is ten times the rate constant for CH4 combustion, the surface temperature near the inlet (1-mm in) is 871.5 K (1100F) and near the transport limit for C7H14 and 823.2K (1050F) and surface rate controlled for CH4. If this calculation is repeated for a series of steps downstream with corrections to the gas phase concentrations and temperatures, new surface temperatures and rates can be calculated through the length of the monolith.

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